

# **Advances in Experimentation & Computation of Detonations**

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# Advances in Experimentation & Computation of Detonations

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Abstracts of the papers submitted to the International Colloquium on  
Advances in Experimentation & Computation of Detonation, St. Petersburg,  
Russia, September 14-17, 1998, are edited and assembled together in this  
volume. Presented are the recent advances made in understanding detonation  
wave initiation, propagation, mitigation, and control through experimental  
and computational studies. The volume is intended to be a tool to explore  
the present state of the art, and an avenue for further follow-up for the  
researchers and practicing engineers.

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## FOREWORD

Demands on engines used for propulsion and stationary power are increasing, since current applications involve extreme operating conditions and wide variations in load. While performance is the key focus on propulsion engines, fuel cost and hence lower specific fuel consumption is the driving factor for stationary engines. Though piston engines are extensively used, gas turbines have taken the lead as primary engines for air, sea and land power plant operations. It is time to focus our attention on alternate engine concepts. Considering the rapid energy release, flexibility, easy scalability, and low fuel consumption, engines based on pulsed detonation waves offer a significant potential. Further multi tube detonation engine with controlled sequential detonations might provide thrust vectoring without external mechanisms.

Though detonation phenomena and its various aspects have been studied extensively over the past several decades, and have been utilized in devices, application of detonation to propulsion or stationary power engines is not yet realized. There has been a global resurgence on applied detonation research focussing on propulsion engines. However funds for research and development have been frugal globally, and have been decreasing. So it is timely and appropriate to review the accomplishments in detonation research, disseminate the current state of the art, and to plan for future cooperative efforts that can bring back substantial return for research investment. With this in mind, we have organized the International Colloquium on Advances in Experimentation & Computation of Detonations.

It is our hope that this Colloquium will provide an open forum for discussions and exchange of ideas and methodologies, but above all lead to joint research efforts on a global basis. Response to present papers and participate in the Colloquium has been very encouraging. An edited Book of Abstracts is made available to the participants. Selected papers will be edited and will be made available as a book in a few months. The U.S. Office of Naval Research (ONR)\*, ONR International Field Office Europe\*, European Research Office of the U.S. Army\*, Combustion Council of the Russian Academy of Sciences, Russian Foundation for Basic Research, and ENAS Research & Education

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\*The content of the information does not necessarily reflect the position of the United States Government and no official endorsement should be inferred.

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Company are jointly supporting this Colloquium. This is an indication of the interest in detonation phenomena.

We like to thank Dr. Sc. S.M. Frolov, Prof. N.N. Smirnov, and Dr. K. Kailasanath for taking the responsibility on technical matters. Our thanks are also due to Dr. Sc. Yu. A. Gordoplov and Ms. Julia Vinyarskaya for local arrangements, and to Ms. Irina Serova and Ms. Olga Frolova and the ENAS staff for the organization of this Colloquium, and the publication of the announcements, book of abstracts and the forthcoming book.

We wish that this Colloquium will be able to offer you a rewarding scientific experience, as well as a time to remember in the years to come.

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Russia

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*September 1998*

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## INTRODUCTION

Almost a century ago, in 1899, Chapman provided a theoretical estimate for the detonation velocity based on one-dimensional flow considerations and compared it with experimental data. Since then, significant progress has been made both in the experimentation and computation of detonations. This international Colloquium is organized to provide a forum to assess the state-of-the-art and a means to disseminate this information to the international scientific community.

Although the study of detonation phenomena has been active during the past century, the application of detonations for non-destructive purposes, such as propulsion, drilling, pressing, protective coating, etc., has been studied only in the past few decades. It is hoped that recent advances, captured in this volume, will provide an additional impetus for the application of detonations for propulsion. With this point of view, though the topics covered in the Colloquium emphasize basic understanding of detonation initiation, structure, propagation, mitigation, and control, it is anticipated that the discussions will focus towards making use of this basic understanding of detonations for applications to propulsion.

The book includes 75 contributions addressing various aspects of detonation physics and chemistry, submitted by researchers from Algeria, Belgium, Canada, France, Germany, Japan, Poland, Russia, Ukraine, United Kingdom, and the United States of America. Of the papers selected for oral and poster presentations, thirty eight (38) papers provide new information gained from experiments, and out of these nine (9) include theoretical models of the phenomena under study. The remaining thirty seven (37) papers are purely theoretical or computational and provide additional information on advances in the physics and applications of detonations. From the response of researchers, there seems to be a balance in the experimental and computational studies carried out.

Section **Detonation Initiation** includes contributions on the most challenging problem in detonation physics. Experimental and theoretical studies on initiation of gaseous and heterogeneous detonations are presented. The issues addressed are the critical energy of detonation initiation (Borisov, Vasil'ev et al., Vidal and Khasainov, Wilson et al.),

deflagration-to-detonation transition (DDT) (Borisov, Smirnov et al., Subbotin, Ilyin and Abruks), enhancement of DDT (Borisov, Rose et al., Wilson et al., Subbotin, Bartenev et al., Gelfand et al.), transition of confined detonations into unconfined ambience (Borisov, Manzhaley), detonation initiation in suspensions of high explosives (HE) in air (Grigor'ev et al.) and vacuum (Zhdan and Prokhorov), and the use of advanced algorithms for computing transient flows with non-reactive and reactive shock waves (Rose et al., Smirnov et al., Gelmeyr, Bartenev et al.). Wilson et al. and Smirnov et al. discuss the applicability of various concepts of detonation initiation to Pulsed Detonation Engines (PDE) and Pulse Detonation Generators, respectively.

Section **Detonation Wave Structure and Propagation** includes contributions on experimental and theoretical studies of detonation structure and propagation mechanisms in gaseous and heterogeneous media. The issues addressed are the multi-dimensional structure of self-sustaining gaseous detonation fronts (Oran, Hanana et al., Hayashi, Sharypov, Rybanin, Trotsyuk, Gvozdeva and Scherbak), transition from regular to irregular cellular patterns (Sharypov, Rybanin), detonation cell structure and size (Oran, Hanana et al., Nikolic et al., Hayashi, Gavrikov et al.), structure of self-accelerating flames (Gostintsev et al.), oblique detonation wave structure and stability (Viguier and Desbordes), gaseous detonation propagation and structure in tubes of variable cross section (Baklanov et al.), anomalous phenomena in shock-plasma interactions (Basargin and Bedin), and the propagation and structure of combustion and detonation waves in porous media (Korzhasvin et al., Pinaev). Baklanov et al. discuss the advantages of their approach for utilization in practical applications, such as propulsion devices.

Presented in Section **Detonation Mitigation and Control** are the contributions on experimental and theoretical aspects of gaseous and heterogeneous detonation control by various means, namely, by changing composition and density of the reactive mixture (Mitrofanov, Auffret et al., Khadyev and Starikovskii, Sychev), by obstructions and wall inflections (Mitrofanov, Fisher et al., Gelfand et al., Kopchenov et al., Galburt and Ivanov), by preliminary vibrational excitation of reactive mixture (Starik and Titova), and by electrical discharge (Afanas'ev et al.). Also addressed are the fundamental issues dealing with stability of a planar detonation wave (Williams), detonability limits (Aslanov and Lubchenko, Sychev), the effect of combustion generated pressure waves on turbulence (Luo), geometrical scaling of flame acceleration and DDT in obstructed ducts (Kuznetsov et al.),

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controlling pre-detonation distances during DDT (Sumskoi and Borisov), and deflagration and detonation analogies in superheated liquids (Ivashnev et al.). In a number of papers, the applications of various detonation controlling strategies to practical facilities are discussed. In particular, Mitrofanov considers such applications as non-electric means for explosion initiation, and controlled detonation of propellants in power plants and jet engines, Kopchenov et al. discuss controlling strategies in scramjets with detonation combustion and ram accelerators.

Section **Applications of Detonation Phenomena** deals with contributions on detonation applications in propulsion (Zitoun et al., Cambier, Levin et al., Kailasanath, Berlyand and Vlasenko), transportation (Korobeinikov et al.), power engineering (Chereshnev et al.), safety engineering (Klemens et al., Zhukov et al.), and processing technology (Baklanov and Gvozdeva, Diachkin and Rybakov). Propulsion applications are focussed towards PDE (Zitoun et al., Cambier, Levin et al.) and ram accelerators (Kailasanath). Korobeinikov et al. consider an internal combustion engine with electrochemical pulse jet ignition followed by detonative combustion. The use of electro-physical properties of detonation products in explosive fast opening switches is suggested by Chereshnev et al. for fast (microsecond duration) energy transmission from explosive magnetic generators to a load. Klemens et al. study the mechanisms of dust explosions in coal mines required for safety regulations. Baklanov and Gvozdeva study the peculiarities of detonation assisted surface depositing of protective coatings based on aluminum oxides. Diachkin and Rybakov investigate explosion pressing of metal powder for obtaining specimens with desired properties.

Section **Detonability of Advanced Fuels** deals with theoretical and experimental studies of detonation properties of various gaseous, heterogeneous, and solid fuels. Detonation of dispersed aluminum in oxygen and/or air is studied by Ingnoli et al., Fedorov et al., Victorov et al., while Imkhovik and Solov'ev consider oxidation of aluminum particles in detonation products of HMX, RDX, TNT, etc. Frolov et al. report a semi-empirical oxidation mechanism of heavy hydrocarbon fuels — prospective candidates for applications in PDE. Jet combustion of hydrogen as a prospective fuel for propulsion devices is studied by Baev et al. Azatyan et al. study the effect of gas-phase inhibitors on hydrogen-air detonations. Fomin et al. report a model of hydrogen combustion in a bubble detonation wave. DDT and the mechanisms of convective burning and low-velocity detonations

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## Introduction

in porous propellants are studied by Sulimov and Ermolaev, Ischenko and Khomenko, and Imkhovik et al. Mitrofanov and Subbotin report the results of experiments on detonation of deposits of HE (lead azide, PETN, RDX) particles in evacuated tubes, and Zhdan and Prokhorov suggest a theory of detonation of RDX particle suspensions in ducts. Detonability of liquid explosives such as nitrobenzene and propynol is studied by Kozak and Kondrikov, and hydrazine by Voskoboinikov and Victorov et al. Another contribution by Victorov et al. presents thermodynamic calculations of detonation parameters of *n*-propylnitrate, nitromethane and a number of other fuels. Experimental techniques for determining burning and gas formation laws in condensed systems are described by Khomenko et al. Abruikov and Ilyin analyze various optical methods for detonation studies.

It is evident that a great deal of research is going on around the world focussing on this interesting phenomenon — detonation. It is our sincere hope that this book will help in formulating a dialogue among the members of the research community.

*Editors*

# DETONATION INITIATION

## INITIATION OF DETONATION IN GASEOUS AND TWO-PHASE MIXTURES

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Diverse aspects of initiation of detonation in gaseous mixtures, liquid fuel sprays, and suspensions of solid particles primarily in air are discussed. The emphasis is made on the following problems.

- (1) Direct initiation of gaseous detonation in ducts, including the following measurements: the minimum initiation energy, its dependence on the rate of energy deposition, density of the initiator, effect of chemical promoters and inhibitors, dependence of the detonation limits on the initiation energy, and shock wave-to-detonation transition.
- (2) Direct initiation of detonation in unconfined clouds of various geometry, including a derived correlation between the initiation energies of plane and spherical detonation.
- (3) Transition of detonation from ducts into unconfined mixture volumes.
- (4) Experimental and theoretical approaches to estimating the initiation energies (the use of detonation cell size and direct kinetic data in calculations is discussed).
- (5) Direct initiation of detonation in liquid sprays (experimental and hydrodynamic codes used to predict the minimum energy of initiation are considered, with particular attention paid to the kinetics of heat evolution behind shock fronts in these two-phase mixtures).
- (6) Direct initiation of dust suspensions of both low- and high-density, with and without solid oxidizers added.
- (7) The effect of premature burning of liquid and solid fuels on the initiation of detonation or deflagration-to-detonation transition (DDT).

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#### Detonation Initiation

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- (8) The mechanism of DDT and the methods for shortening pre-detonation distances in all systems.
- (9) Detonation initiation with injection either of hot reactive gases or self-igniting additives.

A conclusion is drawn that initiation of detonation can be facilitated by the following: addition of some chemical promoters, injection of hot gases or chemicals that produce temperature and concentration gradients, and by enhancing turbulence. In heterogeneous mixtures, the powerful factor affecting detonation onset is ignition or preheating of the condensed particles before sending the initiating gasdynamic pulse.

## INITIATION OF GASEOUS AND HETEROGENEOUS SYSTEMS

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Large-scale accidents with explosions of gaseous or dispersed condensed fuel have attracted the attention of researchers from many countries.

In the present paper, the modern state-of-the-art of theoretical and experimental research on 'direct' initiation of various homogeneous and heterogeneous systems is discussed.

For gaseous fuels, three classes of models are analyzed allowing to determine the critical initiation energy of detonation:

- (1) numerical models based on the joint solution of the one-dimensional equations of gas dynamics and chemical kinetics;
- (2) approximate models based on the idealized scheme of a detonation wave (DW);
- (3) approximate models which are taking into account the real multifront DW structure.

For gas - fuel droplet systems, the physico-mathematical models of DW initiation are analyzed which account for the dynamics of droplet deformation and breakup, the ratio of characteristic times of gas dynamic and chemical processes, droplet sizes, etc.

The large amount of computational information is used to make a quantitative comparison of various initiation models and to present their agreement with available experimental data. For this purpose, experimental data obtained in research centers in Russia, Canada, USA, France, Norway, England, and Germany were used. The analysis indicates that the initiation models developed by the authors provide the best agreement with available experimental data.

On this basis, the dependencies of critical initiation energy vs. fuel concentration were plotted for various fuel-oxygen and fuel-air mixtures which are then used to determine their comparative explosive hazard under planar, cylindrical, and spherical initiation.

## INITIATION OF ADIABATIC EXPLOSION BY ACCELERATED CURVED SHOCK: A THEORETICAL AND NUMERICAL STUDY

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A theoretical and numerical study on the initiation of adiabatic explosions by accelerated curved shocks in homogeneous explosives is presented, with special attention paid to the critical conditions for initiation. The characterization of the response of a reactive substance to a compression by a shock is important to the understanding of problematic events, such as the shock amplification by the chemical heat release and the transition to the detonation regime.

Most homogeneous substances decompose according to a two-stage mechanism, induction and explosion. Induction is the period of time when the reaction progress variable remains small. This stage is described here by the one-step forward irreversible Arrhenius reaction rate. The induction time corresponds to the rapid growth of the dependent variables or, mathematically, to a logarithmic singularity in the material distributions of the dependent variables. In the induction zone, these distributions are expressed as first-order expansions in the reaction progress variable about the shock. Then, the framework of the procedure is the formal Cauchy problem (initial-values problem) for quasi-linear hyperbolic sets of first-order differential equations, such as the balance laws for adiabatic flows of inviscid fluids considered in this study: when a shock front is used as the data surface, the solution to the Cauchy problem yields the flow derivatives at the shock, thus the induction time, as functions of the shock normal velocity and acceleration,  $D_n$  and  $\delta D_n/\delta t$ , and the shock total curvature  $C$ . Next, a necessary condition for explosion is derived as a constraint among

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$D_n$ ,  $\delta D_n/\delta t$  and  $C$  that ensures bounded values of the induction time. This criterion is an illustration of Semenov's hypothesis, namely, the critical condition for explosion to occur is that the heat production term just exceeds the loss term. Here, the production term is the chemical heat release rate and the (adiabatic) loss term is governed by a combination of  $D_n$ ,  $\delta D_n/\delta t$  and  $C$ . The violation of the criterion defines a critical shock dynamics as a relationship among  $D_n$ ,  $\delta D_n/\delta t$  and  $C$  that generates infinite induction times. Depending on the rear boundary conditions, which determine the shock dynamics, this event can be interpreted as either a non-initiation or the decoupling of the shock and of the flame front induced by the shock.

The approach is illustrated by a simple analytic solution to the problem of the initiation by impact of a non-compressible piston. From the continuity constraint in the material speed and acceleration at the contact surface of the piston and the explosive, the dynamics of the shock induced in the explosive is derived and then the induction time and the initiation condition are rewritten in terms of the piston speed, acceleration and curvature. These theoretical results are finally compared with those of our direct numerical simulations in the case of impacts on a gaseous explosive by planar or curved, constant-speed or accelerated pistons.

## AMR CALCULATION OF IGNITION AND DETONATION FORMATION IN REACTIVE GAS BY SHOCK WAVE FOCUSING

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Shock and pressure waves can propagate into reactive mixtures without causing any significant ignition or subsequent reaction activity. If such waves are reflected and focused by curved surfaces, a region of high energy density near the gasdynamic focus is formed, where explosive reactions can start [1]. Therefore, shock wave focusing has been applied in a great variety of scientific [2-4] and engineering applications [5].

In the present work, the focusing process leading to the ignition of a stoichiometric  $H_2/O_2$  mixture is investigated by numerical simulations based on the reactive Euler equations in two dimensions. The computational setup is similar to a circular reflector, which is connected to a rectangular shock tube, as used in [5]. An operator splitting technique is applied to handle fluid flow and chemistry separately. The convective part is integrated using the Harten-Yee TVD method and the integration of chemical source terms is performed by an explicit Euler method. A one-step reaction mechanism is used to model the chemistry of the premixed gases and adaptive mesh refinement (AMR) is applied to get an adequate resolution of steep gradients especially in the ignition and reaction zones of the combustion process.

Calculations are performed for incident shock Mach numbers ranging from 1.7 to 2.2. At lower shock strength,  $M \leq 2.1$ , the complex interaction of reflected shock and expansion waves during the focusing process dominate the wave field, and chemistry is not significant. The computed results show the same wave patterns as obtained by experiments [5] for a similar setup. In the case of higher Mach number of 2.2, the calculations show the ignition of a detonation wave in the focal region, which becomes spherical and interacts with the diffracted shock wave, resulting in an even more complex wave field.

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## **SUMMARY OF GASEOUS DETONATION TUBE EXPERIMENTS AT THE UNIVERSITY OF TEXAS AT ARLINGTON**

**D. R. Wilson, F. K. Lu, and W. S. Stuessy**

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Results from a series of gaseous detonation tube experiments will be presented. The experiments were conducted to develop a better understanding of detonation wave ignition and propagation phenomena in gaseous fuel/oxidizer mixtures. Two detonation tubes were used in the investigation. The smaller tube had an internal diameter of 7.62 cm and was constructed of different length tube segments to permit a variation of the length-to-diameter ratio from 3 to 12. It was constructed as part of a research program to develop a Pulse Detonation Wave Engine (PDE). The second tube had an internal diameter of 15.24 cm and a fixed length of 3 m. It was used as the driver tube for the UTA detonation-driven shock tube facility.

An electric arc ignition system, capable of delivering arcs with energy levels ranging from 2 to 20 J, was used to initiate the detonation process in the 7.62 cm diameter tube. For initial pressures on the order of 1 atm, this energy level was sufficient to directly initiate a sub-critical Chapman-Jouguet (CJ) detonation wave with speeds on the order of 50 percent of the CJ wave speed. The high-energy arc ignition drastically reduced the length required for the deflagration-to-detonation transition (DDT) that is generally observed with low energy igniters. Natural transition to a CJ detonation wave occurred about 23 cm downstream of the igniter for stoichiometric mixtures of oxygen and propane at an initial pressure of 1 atm. However, initial pressures of 2 and 3 atm, respectively, were required for natural transitions to CJ detonations in hydrogen/oxygen and methane/oxygen mixtures. Higher initial pressures caused an earlier transition to a CJ detonation wave. Hydrogen and propane could also be detonated in air, provided the detonation wave was first initiated in a pre-ignition chamber containing the corresponding fuel/oxygen mixture. Turbulence enhancement devices and the use of an annular geometry

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had a significant effect on the detonation wave development, whereas length-to-diameter ratio, ignition energy level and ignition location was of secondary importance. End-wall pressure measurements were made to evaluate thrust potential of various configurations, and results were in general agreement with theoretical considerations. The end-wall pressure level was directly influenced by the speed of propagation of the detonation wave. Downstream ignition resulted in about a 25 percent increase in the integrated impulse imparted to the thrust plate compared to upstream ignition.

Both, arc ignition and shock-induced initiation of the detonation wave were used in 15.24 cm diameter tube. CJ detonations were achieved in hydrogen/oxygen, hydrogen/air and propane/oxygen mixtures, whereas speeds of only 40 percent of CJ wave speed were achieved in propane/air mixtures. Initial pressures up to 8 atm were evaluated, and a number of runs also used various amounts of helium dilution. In general, results were in agreement with the simple Zeldovich-von Neumann-Döring (ZND) model. The shock-induced detonation (SID) mode produced much higher driven-tube performance than the arc-ignition mode. In the SID mode, a 41.3 MPa (6000 psi) helium driver was placed upstream of the detonation tube, and the shock wave initiated by rupture of the intervening diaphragm quickly transitioned to a CJ detonation wave. By proper tailoring of initial conditions, the tube could be operated in the 'perfectly-driven' mode whereby the Taylor rarefaction wave associated with the arc ignition mode could be essentially eliminated. This produced a much stronger shock wave in the driven tube for comparable pressure levels. Driven-tube shock Mach numbers of 11 have been obtained for the SID mode.

## **SOLVING CHALLENGING PROBLEMS IN SHOCK PHYSICS WITH TITAN**

**M. Gehmeyr**

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Under the auspices of the Laboratory for Computational Astrophysics the implicit adaptive grid code TITAN for solving problems in hydrodynamics, radiation transfer, and radiation hydrodynamics has been developed and disseminated. In this presentation, it is shown how two very challenging problems in shock physics can be solved.

First, 'constant velocity shock problem' [1] is discussed. The solution is constructed in planar, cylindrical, and spherical geometries numerically by employing the adaptive grid algorithm and the corresponding (exact and approximate) analytical expressions are derived.

Second, the investigations of the 'sub- and supercritical shock problem' [2] is presented. In a parameter space study, the transition of a radiatively driven shock from the subcritical to the supercritical regime was considered. This allowed to improve the Zel'dovich non-equilibrium diffusion analysis and derive more accurate relations.

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## STUDY OF THE PROCESS OF DEFLAGRATION-TO-DETONATION TRANSITION IN GASES AND ITS APPLICATIONS

N. N. Smirnov, V. F. Nikitin, A. P. Boichenko, and  
M. V. Tyurnikov

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The results of experimental and theoretical investigations of deflagration to detonation transition (DDT) in hydrocarbon-air gaseous mixtures are presented. Multiple scenarios of DDT in methylene cyclopropane ( $C_4H_6$ )-air mixtures were observed. Flow was visualized using a schlieren method with a laser light source. It was proved that the two major scenarios of DDT, discovered by Oppenheim, Soloukhin, Salamandra and their co-workers for hydrogen-oxygen mixtures, were also typical for hydrocarbon-air mixtures. Besides, several other mechanisms of the onset of detonation in the flow which is precompressed by the accelerating flame were discovered. Thus, five unique scenarios were distinguished.

First: the detonation wave can be traced from the flame zone. The wave accelerates rapidly in the precompressed gas and, after interaction with the overtaken leading shock, forms the overdriven detonation wave in undisturbed mixture and then gradually decays to the Chapman-Jouguet (CJ) mode.

Second: the onset of detonation takes place on one of flow non-uniformities (contact discontinuities) ahead of the flame in the precompressed gas between the leading shock and the flame zone (the classical 'explosion in the explosion'). This local explosion gives birth to both detonation and retonation waves.

Third: spontaneous flame propagating in all directions at a high apparent velocity appears in the non-uniformly precompressed gas between the flame zone and the leading shock, that finally brings to formation of both detonation and retonation waves.

Fourth: the secondary combustion zone originates in the precompressed gas ahead of the main flame zone due to autoignition on a contact surface with flame propagating in both directions at a normal burning velocity similar to that in the main flame. That finally leads to formation of detonation and retonation waves in the long run.

Fifth: ignition takes place locally on flow non-uniformities in a number of spots in the precompressed gas ahead of the main flame zone practically simultaneously. Those ignition events give birth to flame zones expanding on both sides. The increase of the flame surface and energy release per unit volume leads to a rapid pressure increase and formation of detonation and retonation waves. The flow pattern macroscopically looks like a volume explosion or a fast spontaneous flame; but on refining the resolution one can see a stochastic ignition time shift from one hot spot to another. The sequence of ignitions is also stochastic that testifies the fact that autoignitions in different hot spots take place independently and do not form a succession or belong to one chain process.

Mathematical modeling of DDT in viscous heat-conductive chemically reacting mixtures was performed wherein chemistry was modelled by a two-step kinetic mechanism. The first step is the induction reaction without energy release, and the second exothermic stage proceeds upon completion of the first reaction. To take into account the initial small scale turbulence, the two-equation  $k$ - $\epsilon$  model is used. The numerical method allows to simulate deflagration and detonation processes, flame front acceleration, DDT, and large scale transverse oscillations of the detonation wave.

Numerical modeling shows that actually the core of the process is the thermal explosion taking place at the contact discontinuity that can develop rather rapidly to a detonation mode, or it can develop in a slower combustion mode providing enough time for other hot spots to reach autoignition. Thus, the different state of the precompressed gas ahead of the flame creates the detected multiplicity of DDT scenarios.

Theoretical studies of a multi-dimensional process of the onset of detonation show that the accelerating turbulent flame influenced by compression waves reflected from the walls of a closed vessel has an unstable structure. This large scale instability gives birth to strong non-uniformities of energy release in the reaction zone. The non-uniformities lead to non-uniform flow and hot spot formation either in the vicinity of the flame zone or ahead of it in the precompressed gas. Sequential thermal explosions in the hot spots result in spherical detonation waves overtaking the leading shock. Thus a structure with relatively large irregular cells can be formed in the first stage of DDT.

Theoretical and experimental investigations of DDT characteristics in hydrocarbon-air mixtures were used to develop a pulsed detonation wave generator with periodic stable detonation waves arising with a frequency of 10 Hz.

## **RAREFACTION WAVE AS A START IMPULSE FOR TRIGGERING EXPLOSION BY THE FLAME ESCAPE THROUGH THE ORIFICE INTO THE CHAMBER**

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The processes of deflagration-to-detonation transition in gaseous combustible mixtures may be greatly facilitated, when obstacles are placed in the path of the flame. Similar phenomena are observed downstream of a pipe or an orifice during exhaust of hot gas into a chamber. In the latter case, the shock waves (SW) propagating ahead of the flame front, decay due to diffraction at the orifice edge and cannot ignite the gas. A possibility of detonation onset in a gas heated by the mixing of hot combustion products with unburned gases, rather than by SW, has been discussed in [1] for the first time. In the present paper, flame propagation through a narrowing path, followed by the formation of an underexpanded supersonic jet of unburned gas, is investigated by the framing schlieren photography. Specific features of the phenomenon become more apparent when the combustion products enter the jet and a rather large 'starting configuration' with a symmetric 'triple lobed' structure arises in a volume. First, the burned gas appears inside the lateral lobes and later in the central lobe. The starting configuration is presumably the unburned gas penetrated by jets of combustion products. Its formation, ignition and explosive combustion occur due to intense mixing of burned and unburned gases in the flow locations with large pressure gradients. The expansion fan with a top located near the rear edge of the orifice is one of those locations. Thus, when the flame emerges from the orifice, the layer of the compressed unburned gas, propagating at a supersonic velocity ahead of the flame, should form. In this case, rarefaction waves and explosions may arise.

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## EXPLOSION INITIATION IN A LARGE VOLUME BY LOW-VELOCITY DETONATION WAVES

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The paper presents the results of experimental studies of transition of gas explosion from one volume to another, through a long capillary by three marginal detonation modes: the high-velocity, galloping and low-velocity modes.

It was discovered, that the gas in the chamber burns out, irrespective of the type of detonation waves propagating in a capillary in the stoichiometric acetylene-oxygen mixture.

Initiation of gas combustion by a propane-oxygen detonation is considerably more complicated. Low-velocity detonation does not ignite the mixture in a chamber under any pressure. Similarly, the galloping detonation does not lead to explosion, if it leaves to a capillary in a phase close to the minimum in the velocity history. Principal differences of these mixtures in terms of gas ignition by detonation are related to a considerable difference in laminar flame velocities. The criterion for gas ignition in a chamber is proposed.

## NUMERICAL MODELING OF IGNITION AND DETONATION PHENOMENA UNDER FOCUSING CONDITIONS

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The initiation of combustion in gaseous media due to the shock wave focusing process at concave reflectors is an important phenomenon, both from the theoretical and practical points of view. A complex gas flowfield coupled with chemical kinetics provides a wide spectrum of possible regimes of combustion, such as fast flames, deflagration, detonation, etc.

The objective of this research is the theoretical determination of critical parameters of combustible mixture as well as the geometry and size of reflectors at which the ignition process and further deflagration or detonation escalation are plausible. The following basic aspects are considered:

- The investigation of a complex wave dynamics inside reflector of a particular type
- Localization of zones of elevated temperature, where ignition can be expected
- Analysis of temperature behavior in these zones from the point of view of ignition kinetics
- Detailed analysis of wave patterns due to the process of flame or detonation propagation

The problem is studied numerically by the solution of a general set of 2D gasdynamic conservation equations together with a detailed scheme of chemical reactions. A special procedure of mesh refinement was used to provide a correct interpretation of boundary conditions at internal curved surfaces of reflectors.

As a basic configuration, a combustible mixture containing 15%  $H_2$  and 85% air was chosen. The flowfields under focusing conditions at the corner and parabolic reflectors were calculated. The angle of corner reflectors varied from  $30^\circ$  to  $120^\circ$  and Mach number of an incident shock wave was in a range 1.5 to 2.5. The focal parameter for parabolic reflectors ranged from 0.17 to 0.5. Thus, initial conditions permit investigation of both regular and Mach reflections on the focusing surfaces.

Verification of numerical results was done on the basis of comparison with experimental data obtained for a definite set of corner and parabolic reflectors.

Systematic numerical calculations showed, that the ignition process is strongly facilitated by the presence of focusing surfaces. Ignition starts at the point of maximum temperature, which does not necessarily coincide with the location of maximum pressure, in the case of parabolic reflectors. The pressure and temperature distribution at a time prior to ignition is very non-uniform. This provides a basis for spontaneous flames to develop at the initial stage of the combustion process and further decay in a structured complex consisting of a shock wave and burning front on later stages. This phenomenon is discussed in terms of mild and strong modes of ignition.

Particular attention is paid to the effect of reflector size on the ignition process under focusing conditions. On the basis of data obtained in numerical calculations, a theoretical model, which describes the influence of scale factor on ignition for corner reflectors is developed.

## DEFLAGRATION TO DETONATION TRANSITION IN $H_2$ + AIR MIXTURES UNDER SHOCK WAVE FOCUSING

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The process of shock wave focusing was investigated in combustible  $H_2$  + air mixtures. The set of experimental measurements was realized for the study of shock waves interaction with concave cavities in modified laboratory shock tubes with round (diameter 54 mm) or rectangular ( $34 \times 50 \text{ mm}^2$ ) cross-section. A cylindrical tube was equipped with three-dimensional (spherical, conical) reflectors, and a rectangular tube was equipped with two-dimensional (cylindrical, wedge) endplates. It was found that the mode of explosion (fast flame, deflagration-to-detonation transition, detonation) behind converging shocks depends on the intensity of wave, hydrogen concentration in the mixture with air and the residence time of combustible mixture in the zone of elevated pressure (temperature) in a convergent flow. The critical conditions of self-ignition were determined for the focusing cavities used. Three-dimensional cavities were found to be the most efficient for self-ignition and deflagration-to-detonation transition in combustible mixtures.

## INITIATION OF CHARGES OF POWDERED HIGH EXPLOSIVES BY OVERDRIVEN GASEOUS DETONATION WAVES

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There is a marginal regime of an explosive decomposition of a substance under weak initiation of charge of powdered high explosives (HE) in low-strength confinement. The time of an initiation delay  $t_i$  of the regime is  $10^{-5}$ – $10^{-6}$  s, the propagation velocity is  $\sim 1$  km/s. The fact that the net rate of condensed phase decomposition sharply increases in this regime is considered to be established. Model experiments of ignition of particle-gas suspension by gaseous detonation waves were performed. The interaction between particles was thus eliminated. The time of particle ignition delay was measured by means of a multi-wave pyrometer. A sharp amplification of deflagration was observed when the initial pressure of gas mixture  $P_0$  exceeded the threshold value  $P_*$ . The measured value of  $P_*$  coincides with the value of the threshold pressure of the marginal regime initiation in the charge.

A mechanism of particle ignition in the marginal regime is proposed. In high-enthalpy gas flow, a melted layer forms on particles. Fragmentation of the layer results in a sharp increase of the surface area and the net reaction rate of HE. Similar to the initiation of the regime, this process exhibits the threshold behavior. Numerical simulation of particle behavior in the gas flow showed that the heating time of melted layer with the thickness sufficient for fragmentation coincided with  $t_i$ .

Experiments on initiation of a charge of powdered HE in low-strength confinement by the overdriven gaseous detonation wave were performed. Dependencies of  $P_*$  on particle diameter and on physical properties of HE were obtained. The experimental data indicate that the shock wave mechanism is unable to initiate the marginal regime. The increase in the net reaction rate of condensed phase decomposition cannot be explained by increasing the HE surface area due to destruction of solid particles. The proposed mechanism of particle ignition is in good agreement with experimental data.

## INITIATION OF RDX AND HMX DUST DETONATION IN VACUUM

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A possibility of high-explosive (HE) dust detonation in vacuum, its structure and propagation mechanisms were discussed in [1]. This paper presents a mathematical model and numerical solutions describing initiation of a detonation wave (DW) in vacuum with RDX and HMX dust. In this model, the unsteady equation of heat conductivity for a particle is coupled with the unsteady two-phase flow conservation equations.

Assume the space  $x > 0$  is occupied by a suspension of monodisperse RDX or HMX particles in vacuum, and the initial mass concentration of the particles  $\rho_{20} = \alpha_{20}\rho_2^0$  and their diameters  $d_0$ . At time  $t = 0$ , the HE particles burn instantaneously in a region  $0 < x < x_*$ . As a result, a high-pressure region of finite dimensions is formed. The initial conditions are as follows

$$\rho_1 = \rho_{20}, \quad u_1 = 0, \quad p_1 = (\gamma - 1)(q_{ch} + c_2 T_{20}), \quad (0 < x < x_*) \quad (1)$$

$$\rho_1 = 0, \quad p_1 = 0, \quad u_1 = u_2 = 0, \quad \rho_2 = \rho_{20}, \quad T_2 = T_{20}, \quad (x > x_*) \quad (2)$$

Under expansion of the initiating region, a non-steady DW can be either initiated or initiation fails and DW decays. Consider the one-dimensional unsteady motion of the cloud of monodisperse particles of volatile HE. When particles are heated by intense flux, the non-uniform temperature distribution  $T_2(x, r, t)$  should be taken into account. It is assumed that, as the surface temperature  $T_{2\sigma} = T_2(x, d_0/2, t)$  attains the evaporation temperature  $T_s$ , forced gasification on the particle surface starts.

**Numerical Results.** The dynamics of initiation of a plane, cylindrical and spherical DW and the approach to steady detonation conditions are numerically determined by varying the following parameters: the length of the initiation region ( $x_*$ ), the mass concentration of dust ( $\rho_{20}$ ), the particle size ( $d_0$ ), and the geometry of problem ( $\nu$ ).

Calculations are performed for RDX and HMX particles. In terms of dimensionless variables and coordinates  $\tau = tq_{ch}^{0.5}/x_0$ ,  $\xi = x/x_0$ , with  $x_0 = d_0^2 \rho_2^0 q_{ch}^{0.5} / 18 \mu_{10}$  ( $q_{ch}$  is the heat of chemical reactions per unit mass of fuel,  $\mu_{10}$  is the dynamic viscosity of gas) chosen as a linear dimension, the solution of the non-steady problem with the initial conditions (1), (2), retaining terms  $O(\alpha_{20})$ , depends only on three dimensionless constants:  $K = \rho_{20} d_0 q_{ch}^{0.5} / 18 \mu_{10}$ ,  $\xi_* = x_*/x_0$ , and  $\nu$ . The critical length of the initiation region  $\xi_{cv}$  with variation of parameter  $K$  is determined for RDX and HMX dust in vacuum. If  $\xi_* > \xi_{cv}$ , an initiating wave accelerates to the self-sustained detonation regime. If  $\xi_* < \xi_{cv}$ , the wave decays and the gasification of HE particles is terminated. With increasing  $K$ , the critical length  $\xi_{cv} = f(K)$  decreases monotonically. The computed critical initiation energy of HMX dust is larger then for RDX dust. The reasons of this effect are discussed.

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## ON A QUANTITATIVE APPROACH TO THE INVESTIGATION OF THE EARLY STAGE IN THE DEVELOPMENT OF DETONATION IN GASES

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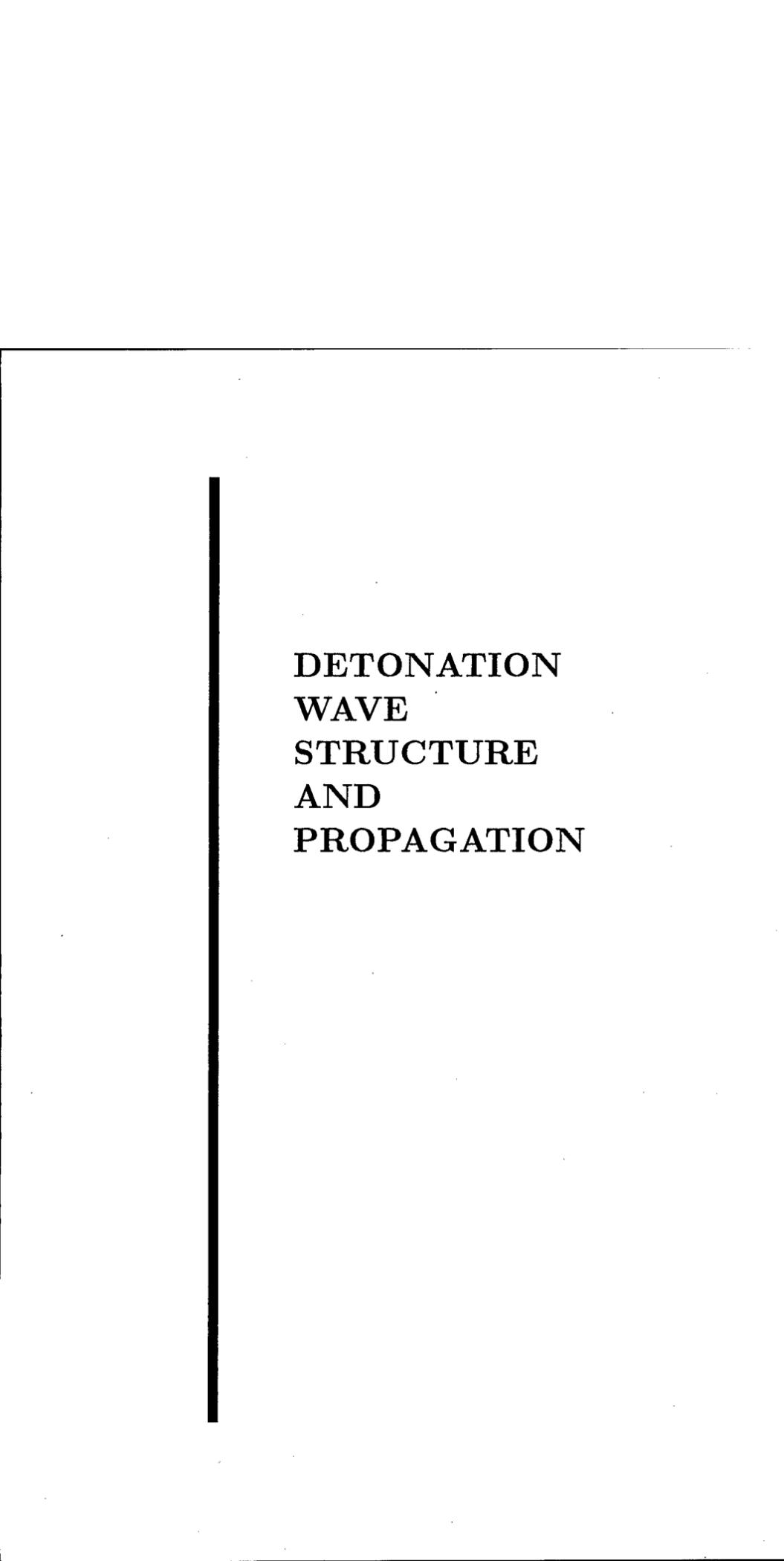
Deflagration-to-detonation transition is a non-stationary gasdynamic process in the development of a new gas flow pattern with shock and detonation formation. According to current concepts, detonation is a process resulting from the cumulation of compression waves associated with accelerated motion of flame, which in turn is dominated by the gas-dynamic processes upstream of the flame.

In [1], the authors proposed an approach allowing commutation of both, the scalar potential of gas momentum density, as well as the velocity field in the potential approximation and the pressure field. The extension of the approach to gaseous detonation allows one to simulate similar profiles for burning and detonating gas.

As far as detonation in pipes is concerned, the approach under discussion makes it possible to determine the cross-section-averaged scalar potential of the momentum density and thereby, the reconstruction of the cross-section-averaged velocity and pressure.

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**DETONATION  
WAVE  
STRUCTURE  
AND  
PROPAGATION**

## THE STRUCTURE OF PROPAGATING DETONATIONS

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It has been known for at least 30 years that the structure of a self-sustaining, propagating detonation is not planar, but consists of sets of Mach stems, incident shocks, and triple points, all of which evolve dynamically as they move through the energetic material. These waves form the diamond-like patterns called detonation cells, whose characteristics, such as size and regularity, are properties of the specific material and the chamber in which the detonation propagates. This presentation describes highlights of what is currently known about the multi-dimensional structure of propagating detonations. Besides being an integral part of the propagation process, the structure has important effects on detonation attenuation: decaying shock waves provide a multi-dimensional mechanisms for quenching detonations. In addition, some of the same factors which affect the detonation structure, such as energy content and distribution, also affect the initiation process. The presentation ends with a brief introduction to new work on deflagration-to-detonation transition.

## ON RECTANGULAR AND DIAGONAL THREE-DIMENSIONAL STRUCTURES OF DETONATION WAVES

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Presented in this paper are the experimental results, that enabled the classification of the three-dimensional structure of the detonation into two fundamental types: a rectangular structure and a diagonal structure. The rectangular structure is well documented in the literature and consists actually of 2 two-dimensional waves. These 2D waves are orthogonal and travel independently from each another. The soot record in such case shows classical diamond detonation cell exhibiting 'slapping waves'. Those structures are not fundamentally three-dimensional but may be described as  $2 \times 2D$ .

The diagonal structure has not yet been reported as such and is characterised by soot record without slapping waves. These structures have been occasionally mentioned in the literature, incorrectly called 'planar mode'. However, the recent experiments indicate that such structure is actual 3D where the triple points are moving along the diagonal line of the tube cross section. The axes of the transverse waves are canted at 45 degrees to the wall, accounting for the lack of slapping waves. Those diagonal structures are the only ones fundamentally three-dimensional. The diagonal structure exhibits a better sustaining mechanism than the rectangular mode. It is possible to reproduce these

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diagonal structures at wall by appropriate control of the experimental ignition procedure. The characteristics of the diagonal structure show some similarities with detonation structure in round tubes. Such diagonal structures have not yet been reported in three-dimensional numerical modeling.

## **FORMATION OF A HIGH-SPEED DETONATING GAS FLOW FROM A DOUBLE-FRONT NON-STATIONARY DISCONTINUITY**

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The conditions of formation of non-stationary complexes from shock waves and flame front during detonation propagation in channels of variable cross-section have been experimentally investigated. The mechanism of detonation formation after the reflection of a non-stationary complex (so-called regime of double-front non-stationary discontinuity — RDND) is described. Two series of experiments were conducted, the first in a straight closed tube filled with oxygen-hydrogen-nitrogen mixture, and the second in an open duct, which is reduced in diameter at the outlet end, filled with methane-oxygen mixture. In the latter case the 'pulsed' mode of detonation combustion has been attained. The influence of pulse frequency of RDND, on the concentration limits was investigated. The ways of stabilization of conditions for RDND formation were considered by creating an additional ignition source for the combustible mixtures. The influence of ignition location, and the time shift between ignition and arrival of a non-stationary discontinuity at this location, was investigated. For a given detonation chamber, the greatest effect was achieved when additional ignition was arranged at distance 20 mm before the contracting section and 50  $\mu$ s prior to the arrival of a shock wave. Current investigations allowed us to obtain RDND with a probability of 0.995, at a pulse repetition rate ranging from 0.5 to 10 Hz. This opens a possibility of utilizing RDND for practical applications, such as propulsion devices.

## **SIMULATION OF DETONATION CELLS IN WIDE CHANNELS**

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Two-dimensional simulations in channel widths ranging from very narrow ones, up to values equal to 100 half-reaction lengths, with single-step Arrhenius kinetics, have been performed. The case with an overdrive parameter of 1.2, dimensionless heat release of 50 (based upon the pre-shock state), a ratio of specific heats of 1.2, and dimensionless activation energy of 10 is studied. This case was previously thought to produce regular cells, but the present results show otherwise, when the channel width is sufficient to support more than one cell. When the channel width is increased further, the number of cells starts increasing, and the average cell size appears to converge to a value independent of the width.

## DETAILED NUMERICAL STUDY ON HYDROGEN-AIR DETONATION STRUCTURE

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The two-dimensional and three-dimensional hydrogen-air detonation structures are studied numerically for quantitative and qualitative observation of the fine dynamics of triple points. Two different detailed chemical mechanisms are checked by comparing predictions with experimental results. The Euler equations are integrated with 9 species and 38 elementary reactions of both forward and backward directions. A mismatch of numerical results and experimental data was observed earlier. However, more detailed three-dimensional studies of detonation structures for a wide range of equivalence ratios are planned.

## CONDITIONS OF ONSET AND STABILIZATION OF OBLIQUE DETONATION WAVES

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The oblique detonation wave is a credible alternative of sustaining combustion at hypersonic velocities. This supersonic combustion can be used either in a detonation airbreathing engine (ODWE, DRAMJET) for hypersonic flight, or in the so-called RAM accelerator for accelerating a projectile at superdetonative velocities.

Presented in this paper are the recent experimental works concerning the establishment of oblique detonation waves in  $H_2 + 2.38\text{Air}$  and  $H_2 + 2.38O_2$  mixtures. Detonation initiation and its stability are the problems of particular interest in this study.

The oblique detonation wave is induced by an oblique shock wave. The technique of the oblique shock tube is used to produce a supersonic wedge driven by a normal Chapman-Jouguet (CJ) detonation wave of a driver mixture. The flow field induced by the wedge is visualized using multi-frame schlieren and Planar Laser-Induced Fluorescence (PLIF) imaging. Besides, the history of establishment and propagating phase of the structure is followed by the smoked foil technique.

To stabilize a detonation wave in an hypersonic flow, the flow velocity must be higher than the CJ velocity of the studied reactive mixture. In the case of  $H_2 + 2.38\text{Air}$  and  $H_2 + 2.38O_2$  mixtures, the minimum flow Mach number is about 5. Oblique detonation waves at Mach numbers  $M = 6, 7.5$ , and  $8.3$  were observed in this mixture (at initial temperature  $T_0 = 293\text{ K}$  and pressure about few  $0.1\text{ bar}$ ).

Detailed analysis of the structure of the initiation show that the oblique detonation wave appears after a certain delay. This delay can be compared, with a good accuracy, with the chemical induction time of the reactive mixture behind the oblique shock wave. The basic configuration of stabilization of the delayed oblique detonation wave is a three waves structure. These three waves intersect at a triple point; the oblique shock wave, the oblique detonation wave and the transverse wave. The transverse wave propagates inside the post-shock

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### Detonation Wave Structure and Propagation

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gaseous mixture. Very close behind the transverse wave, an intense combustion zone is displayed by PLIF images. Smoked foil records provide additional information about the nature of this transverse wave. For  $M = 6$ , this wave is the shock-induced combustion wave. For  $M = 7.5$  and  $8.3$ , it is an overdriven detonation wave clearly shown on smoked foils as fine cellular structure.

Periodic instabilities of the triple point position are observed for long delayed detonations (i.e. for long induction times). These instabilities correspond to periodic explosions behind the oblique shock wave and ahead the triple point structure, giving birth to a new triple point replacing the old one. This transverse wave drives the entire structure of the oblique detonation wave. It is the origin of the structure of stabilization of delayed detonation waves.

## LARGE SCALE SPHERICAL BLASTS OF PREMIXED GASES

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Self-accelerating combustion of spherical volumes of gaseous reactive mixtures at shockless central ignition in soft shells or without shells is studied. Parametric domains of existence of various combustion development scenarios are determined depending on the radius of the gas volume and normal burning velocity, from comparatively slow combustion of buoyant clouds to a self-similar regime of self-accelerating turbulent combustion.

Evolution of compression waves and formation of stable-wave structure of gasdynamic discontinuities under the effect of the spherical piston with the power law of motion, which is equivalent to a self-accelerating flame, are discussed.

Analysis of experimental data of parameters and circulation of acoustic disturbances under combustion of spherical volumes allows to explain possibilities of transition of combustion to detonation for oxygenous mixtures depending on their acoustic properties.

## THEORETICAL DESCRIPTION OF DETONATION PHENOMENA BASED ON THE CONCEPT OF NON-LINEAR WAVE-KINETICS INTERACTION

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The paper is devoted to the discussion of practical problems in studying detonation wave structure and dynamics. The results obtained during the last decade (by A. A. Borissov, O. V. Sharypov, E. A. Pirogov and others), on the basis of a specific approach to theoretical study of detonation phenomena, are analyzed. Specific features of the approach are based on ideas and methods of the self-organization theory. This approach is universal and can be applied to the description and explanation of a wide variety of detonation effects. This approach can be referred to as 'semi-analytical,' because it implies two stages:

- (1) development of an approximate evolution model of a phenomenon,
- (2) numerical simulation of the phenomenon on the basis of the model.

The models take into account dispersion and dissipation properties of a medium, inter-phase transfer, basic non-linear effects, and kinetics of non-equilibrium processes in the system. This allows for the complete description of the non-linear wave-kinetics interaction in the system with an irreversible chemical reaction. Since the model is approximate, it is much more simple for analysis than the original complete system of equations. In some cases, the system of governing equations can be reduced to a single quasi-linear equation in partial derivatives. Such a significant mathematical simplification of the problem allows to derive, in explicit form, the estimations and analytical criteria governing the changes in phenomenon regimes. This also provides qualitative explanations as well as physical mechanisms of experimentally observed effects.

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The stage of numerical simulation serves to illustrate the conclusions derived from the model and to compare quantitatively the predicted results with experimental data. The complexity of this stage is connected with the instability of solution in linear approximation. Nevertheless, these numerical algorithms are more efficient than the solution of the complete system of equations. Furthermore, it is not a problem to test the algorithms, since the approximated evolution models can be reduced, in certain limiting cases, to equations having well-known exact solutions (heat conductivity equation, Burgers equation, Korteweg – de Vries equation, etc.).

While the discussed approach has its own limitations, nevertheless it was successfully used in theoretical studies of the following problems:

- (1) two-dimensional cellular structure of gas detonation waves;
- (2) transition from regular to irregular cellular structure;
- (3) effect of acoustically absorbing channel walls on the limits of self-sustained regimes and on the detonation wave structure;
- (4) spontaneous onset of detonation regimes in systems near the self-ignition threshold;
- (5) mechanisms of occurrence of bubble detonation.

## TRANSVERSE WAVES AT DETONATION

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Presented in the paper is the analytical theory of transverse waves at the detonation front. The transverse wave is considered as a two-dimensional detonation wave propagating along the compressed gas layer, between the shock front of the maternal detonation wave and combustion products. The regular structure of unstable detonation wave is closely connected with the critical detonation size of the transverse wave: a transverse wave follows a previous one at the distance which provides the width of the compressed gas layer before it equal to the critical size mentioned. Such a model allows to give some new interpretations of unstable detonation properties and the appearance of the regular structure in chaos. For instance, both the characteristic size of wave regularities and the critical diameter of unstable detonation is connected with the existence of the critical size of transverse detonation waves.

## CHEMICAL KINETIC PREDICTIONS OF DETONATION CELL SIZES AND DETONABILITY OF HYDROGEN COMBUSTIBLES

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A correlation between characteristic reaction zone widths calculated from detailed chemical kinetic models and experimentally measured or computed detonation cell sizes is analyzed. The objective is to develop a model to estimate the detonation cell sizes on the basis of detailed chemical kinetic calculations. An approach is proposed to generalize this correlation, taking into account the multi-dimensional structure of real detonations. It is based on the characteristic reaction zone width, calculated with initial conditions representative for a multi-dimensional detonation wave. The ratio of the detonation cell size to characteristic reaction zone width (constant  $A$ ) is considered to be a function of two stability parameters (reduced effective activation energy and energy release). The generalization of the correlation between the cell size and reaction zone width is evaluated against experimental data and results from multi-dimensional calculations. An analytical expression is suggested to describe the dependence of constant  $A$  on the stability parameters. On this basis, the detonability of hydrogen combustibles is analyzed. The analysis includes mixtures of hydrogen, oxygen, nitrogen, steam, and carbon dioxide. Special attention is given to compositions and initial conditions different from those studied experimentally.

## ACOUSTIC FIELDS ORIGINATING BEHIND DETONATION WAVE IN GAS MIXTURES

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It is known, that detonation waves in gaseous mixtures, at high initial pressure, have a complex multi-front structure. At the front of the detonation wave, a large number of three wave configurations colliding with each other, are formed. As a result of collisions, new shock waves and contact discontinuities are generated which can, under certain conditions, roll into vortices. Thus, the flow of the hot gas behind the detonation wave exhibits unsteady wave and vortical motions. However, when studying the structure of detonation fronts, the main attention is usually paid to transverse waves and turbulence.

In the present paper, the analysis of a system of acoustic detonation waves is performed. The flow fields behind detonation waves in hydrogen-oxygen and methane-oxygen mixtures at initial atmospheric pressure, obtained experimentally by optical methods, are analyzed. The velocities of propagation of acoustic disturbances relative to the flow have been obtained and compared with calculated values. It has been found, that acoustic oscillations propagate at the frozen sound velocity, without damping on the large distance behind the detonation wave front. This distance is ten times greater than expected from the corresponding theoretical evaluations. The explanation of this fact based on the new treatment of the Chapman-Jouguet condition for a multi-structure wave is suggested.

## SHOCK WAVE PROPAGATION AND FLOW AROUND BODIES IN LOW TEMPERATURE NON-EQUILIBRIUM PLASMA

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When a shock wave or a flying body enters the zone of gas discharge ( $p = 1\text{--}100$  Torr,  $T = 300\text{--}1400$  K,  $T_e = 1\text{--}6$  eV,  $n_e = 5 \cdot 10^{10}\text{--}10^{12}$  cm $^{-3}$ ), the following anomalous phenomena occur: (1) acceleration of the shock wave compared to the shock entering the gas heated to the temperature of discharge plasma, (2) change in the shock wave structure, (3) changes in the flow around the flying body and in aerodynamic characteristics of the body, (4) change in ablation and heat flux to the body, etc.

Discussed in this paper are the results of experimental research of these phenomena in stationary and decaying plasma of air and Ar in shock tubes and in free flight conditions. It was ascertained that the reason for the arising anomalies is connected with peculiarities of sound propagation in non-equilibrium excited media, due to transformation of superfluous energy of internal degrees of freedom into kinetic energy. It was demonstrated that the Mach number  $M$ , based on the velocity of propagation of high frequency sound, can serve as a parameter for modeling the flows of non-equilibrium plasma. The value of this velocity was determined experimentally. This allowed the estimation of gasdynamic parameters behind shock waves propagating in plasma, and to offer a method for estimating the aerodynamic characteristics of bodies flying in plasma. The estimated values were compared with experimental results. The difference in velocities of shock propagation in plasma and in heated gas was used to determine the amount of internal energy transformed into heat.

## NUMERICAL SIMULATION OF A TWO-DIMENSIONAL $\text{H}_2\text{-O}_2\text{-Ar}$ DETONATION STRUCTURE

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In the present investigation, the two-dimensional Euler equations coupled with the Induction Parameter Model (IPM) of chemical reactions [1] are used for numerical simulation of chemically reacting flows. The first (induction) phase in IPM is based on kinetics [2]. The changes in the internal energy and mean molecular weight of the reacting gas mixture, during the second (energy release) phase, are determined by the repro-model [3, 4]. The system of governing equations is closed by the equation of state for the thermally perfect gas.

The set of non-linear equations is solved by applying the upwind finite volume fourth-order MUSCL TVD scheme [5], combined with an adaptive refinement, moving grid algorithm.

The two-dimensional structure of detonation waves (DW) in  $2\text{H}_2 + \text{O}_2 + X\text{Ar}$  mixture in a wide range of initial pressure (0.0866 to 0.405 bar) with a dilution, range of  $0 \leq X \leq 7$ , has been numerically investigated. The computations provide both an excellent agreement of computed detonation cell width with experimental data [6] and a correct description of the cell shape and the roughness of detonation front [7]. In addition, the dependence of an instantaneous value of detonation front velocity on its location along the cell is obtained. This value is in good agreement with experiments [8] and nearly coincides with the similar dependence obtained by numerical simulation [9]. During numerical experiments, the influence of the initiation (by a single or several initiation kernels, symmetrical or asymmetrical initiation) on the established DW cellular structure has been studied thoroughly.

In addition, the changes in DW structure under variation of the channel width have been investigated. The qualitatively different behavior of two-dimensional DW structure for the mixtures exhibiting (in experiments) a well-shaped detonation cell ( $X \neq 0$ ) and those with irregular structure ( $X = 0$ ) was revealed.

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## NUMERICAL INVESTIGATION OF DETONATION WAVE REFLECTION FROM A WEDGE

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Numerical studies were performed on the propagation of the non-stationary two-dimensional cellular detonation wave (DW) over a wedge, in a flat channel filled with the  $2\text{H}_2 + \text{O}_2$  mixture, at an initial pressure of 0.2 bar. The computational approach is similar to that adopted in [1].

For the Mach reflection of DW, the numerical simulation reveals the essential features of the Mach stem (MS) and its growth as DW propagates along the channel. Despite that MS is the overdriven DW, the use of a high-order accurate scheme resolves its multi-cellular structure. The obtained results of MS behavior are qualitatively similar to experimental observations and numerical simulation [2].

However, distinct from [2], the present work reveals (apparently for the first time by numerical simulation of detonation flows) that MS growth is not self-similar (i.e. the triple point trajectory is not a straight line). This agrees with experimental results [3]. At high values of  $L/a_0$  ( $L$  is the distance along the wedge surface from its apex to MS,  $a_0$  is the cell width in incident DW), the growth of the MS height slows down attaining some limiting value, oscillates around it under the influence of transverse waves coming from the incident DW.

According to the present numerical experiment, a critical wedge angle of transition from regular to Mach reflection is  $52^\circ$ . This value is close to  $50^\circ$  reported in [4]. The flow analysis by the shock polar method for the chemically non-reactive shock wave moving in the specified mixture at the Chapman-Jouguet velocity, gives the angle  $50^\circ 17'$ .

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## ON ONE REGIME OF LOW VELOCITY DETONATION

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The steady-state propagation of combustion waves in inert porous media is possible in various regimes. They differ by the mechanism of propagation, wave structure, and the range of propagation velocities. Among these regimes, a group of detonation regimes is particularly known. They can conditionally be divided into three groups according to the mechanism of propagation and characteristic velocities.

A normal detonation wave with heat and momentum losses propagates at velocities from the Chapman-Jouguet value to about 1500 m/s. The low velocity detonation propagates at velocities from 1500 m/s to 800 m/s, and the slowest detonation regime is the regime of sonic velocities (SVR).

Little investigation was performed on the latter regime. However, burning of a combustible mixture in this regime occurs at the elevated pressure in a wave, similar to other regimes. The pressure at the wave front grows smoothly rather than abruptly. Pressure and temperature rise in the wave is not sufficient to ignite the mixture with short delays, neither in an incident wave, nor after its reflection from the elements of a porous medium or at shock diffraction. A characteristic velocity of such wave ranges from 100 m/s to 800 m/s.

In the present communication, the SVR is considered. The results of experimental investigations on the dependence of flame propagation velocity on the composition of hydrogen-air mixture, in low porosity beds (porosity  $\epsilon = 0.46$ ), open-cell polyurethane ( $\epsilon = 0.98$ ), and some other porous media are discussed. The hypothesis about the mechanism of flame propagation in SVR is justified. It is suggested that the transfer of chemical activity in the wave occurs by convection

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of burning gas jets rather than by the induction mechanism. The flame velocity is controlled by the fastest jets where combustion is still possible under hydrodynamic quenching of flame owing to its stretch. Thus, the hydrodynamic flame quenching at the fastest jets plays the role of a factor that stabilizes the wave velocity at a particular level. The theoretical conceptions developed are in qualitative agreement with experimental data. The nature of limits of existence of this regime is also considered.



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**DETONATION  
MITIGATION  
AND  
CONTROL**

## THE WAYS OF EXPLOSION CONTROL

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The basic methods of explosion control were established earlier. The present paper reviews modern achievements on the problem as it relates to the author's own scientific interests.

The main practically interesting parameters of explosion are the detonation velocity  $D$ , total energy release, and pressure impulse. Explosion can be readily controlled by varying the composition of explosive charge, charge density and its physical structure (for heterogeneous systems). As compared with trivial possibilities of changing the parameters of ideal detonation (within known constraints), non-ideal detonation shows essentially wider range of controlling measures.

The increase in  $D$  by 1.5–2 times and even more, as compared with the Chapman–Jouguet velocity  $D_{CJ}$ , can be achieved in heterogeneous systems if specific conditions for the fast transition of an initiating pulse are created. In particular, it concerns tubes with a layer of a high explosive on side walls and suspensions of particles (not too small) of such an explosive in a light gas or vacuum.

The widest range of changes in  $D$  at  $D < D_{CJ}$  (reduction by 5 and more times) is attained in gas mixtures placed into inert porous media due to gradual increase of momentum and energy losses from the reaction zone. Governing parameters are the pore size, initial pressure, and species concentrations. The transition to low detonation velocities is accompanied by the change in the detonation mechanism. Approximately the same range of reduced  $D$  is realized in bubble media.

In general, by varying composition and heterogeneous structure of explosive charges it is possible to nearly continuously change the propagation velocity of a self-sustaining explosion wave from rather small values of about 10 m/s to 10–14 km/s. A wide range of density change (50–200 kg/m<sup>3</sup>) is possible for heterogeneous explosive mixtures based on superlight polystyrene foam. Detonation of such mixtures has been investigated insufficiently and shows a number of interesting features.

## 'NON-IDEAL' DETONATION MODES IN INERT POROUS MEDIUM

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Presented here is the review of the author's experimental results on detonation of gaseous mixtures, heterogeneous systems (liquid/solid fuel film — gaseous oxidizer) and powder explosives in an inert porous medium with fuel films and powder explosive layers uniformly covering the particle surfaces. Investigations were carried out within wide ranges of particle sizes 0.001–10 mm, initial gas pressure from vacuum to 10 MPa, species concentrations, contents, and types of fuels and explosives.

A number of new processes ('fast' combustion of gas mixtures, 'vacuum' detonation of low-density explosives) were discussed. The classification of all possible detonation and combustion modes is presented. It is shown that the wave front velocity for all the stationary processes is determined by initial parameters of the medium. The reproducibility and variety of combustion and detonation modes in a porous medium is determined by its geometric similarity, the influence of heat loss and the dispersion of sound velocity in a medium. For gaseous combustible mixtures in a porous medium, the increase in initial pressure allows to obtain a nearly continuous range of stationary wave velocities from 0.1–10 m/s to the Chapman–Jouguet detonation velocity (1.5–2.5 km/s). There exist mixtures of fixed content which exhibit smooth or abrupt transitions from combustion to detonation with increase in the initial pressure. The thermal model of limits allows estimation of critical parameter values based on the Peclet criterion.

It follows from the experimental data, that the considered low-velocity detonation modes are non-ideal, since friction and heat losses are rather high; the flow in the reaction zone is chemically, thermodynamically and physico-chemically non-equilibrium; the flow structure in the reaction zone is essentially non-one-dimensional; and the mechanism of detonation ignition and propagation is not shock-induced. The velocity of stationary detonation can continuously decrease to attain

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400–800 m/s near the limit, which is 1.5–4 times lower than the ideal detonation velocity. However, within the whole range of detonation existence and for all the investigated systems, the front of luminescence is situated in the immediate vicinity of the detonation front, and the ignition delay in the front accounts for only a few microseconds, which is 2–3 orders of magnitude lower than the chemical induction period, corresponding to the same detonation velocity value. Such a remarkable resistance (stability) of detonation process is caused by reorganization of the ignition mechanism and the presence of the jet-convective ignition mechanism at detonation limits, when the hot jet velocity at the front is close to the detonation wave velocity.

Another way of controlling explosion is based on external forcing the detonation wave by mass, momentum, and energy fluxes. In this case, a detonation wave becomes also non-ideal. This approach is less investigated, than the first, but ultimately allows to change detonation parameters in a narrower range. It is used for detonation damping and its applicability is restricted by certain critical levels of external forcing. There exist different approaches to determine qualitatively such critical levels of forcing.

The third way of explosion control deals with the geometrical influence on the detonation wave by designing channels of a special configuration. In particular, these are the channels with obstructions of variable blockage ratio and annular channels for attaining continuous spin detonation.

The following possibilities of practical use of explosion control are considered:

- (1) Transmission of a pressure, themperature, or flame pulse at a required propagation velocity (non-electric means for explosion initiation, special engineering and technology);
- (2) Control of explosion effect in technological applications;
- (3) Reduction in explosion hazards of accidental explosions;
- (4) Controlled detonation of propellants in power plants and jet engines.

## THEORY OF MULTI-DIMENSIONAL DETONATION INSTABILITY

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Multi-dimensional instabilities of planar detonations that lead to cellular structures are addressed by use of a distinguished limit in which the propagation Mach number is large and the difference between the specific heats at constant pressure and at constant volume is small. In this limit, the Neumann-state Mach number is small, and the fractional variations of the pressure change after the Neumann state also are small for the overdriven conditions that are considered, under which the heat release is comparable in magnitude with the thermal enthalpy at the Neumann state. The resulting post-shock flow is quasi-isobaric in the first approximation. From the resulting dispersion relation, it is shown that there always exists a transverse wavelength range over which the planar detonation is unstable, independent of the strength of the temperature dependence of the heat release rate, except under extremely highly overdriven conditions.

## EFFECT OF SCALE ON THE ONSET OF DETONATIONS

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Results of deflagration-to-detonation (DDT) tests at two different scales (50 times) and similar geometry are presented. Large scale tests were made in RUT facility [1, 2]. The experimental volume consisted of three parts: first channel of  $2.5 \times 2.3$  m cross-section and 34.6 m length, a room of  $6 \times 2.5$  m cross-section and 10.5 m length, and the second channel of  $2.5 \times 2.3$  m cross-section and 20 m length. There were twelve concrete obstacles located along the first channel 2.5 m apart. The blockage ratio (BR) was 0.3. Small scale tests were made in MINIRUT apparatus which was constructed to simulate the RUT-geometry at 1 : 50 scale. Flame acceleration in a channel with a number of obstacles (BR = 0.3) and critical conditions for DDT both in the channel and in the room were investigated. Mixtures tested in the RUT were hydrogen-air at about 285 K and hydrogen-air-steam at about 375 K. Hydrogen-air mixtures at about 285 K were used in the MINIRUT apparatus.

Flame acceleration in the small scale tests was found to be less efficient compared to that in the RUT tests. With the mixtures, which were close to estimated critical compositions for DDT, the flame acceleration did not result in the choked flames in the MINIRUT apparatus. In order to make the scaling of the critical conditions for the onset of detonation more accurate, special efforts were undertaken to achieve maximum possible speeds of turbulent flame propagation prior to DDT in the MINIRUT apparatus.

A series of experiments was made to determine critical conditions for DDT in the channels and in the rooms of RUT facility and MINIRUT apparatus. It was found, that for the variety of mixtures tested in the RUT (including hydrogen-air-steam with steam concentrations from 5 to 45% vol. at 375 K), the critical compositions for the onset of detonations have similar values of detonation cell sizes  $\lambda$ . The critical values  $\lambda$  were found to be 0.9 m (obstructed channel) and 1.2 m (room) at the scale of RUT facility. In the MINIRUT apparatus, the critical

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hydrogen concentrations for DDT turned out to be 25% in the channel and 24% in the room. The corresponding cell sizes (18 and 21 mm) were found to be 50–57 times smaller than those in the RUT tests. This is a very convincing demonstration in that the minimum ratio of characteristic scales (geometrical length scale over chemical length scale  $\lambda$ ) necessary for the onset of detonations is constant over a wide range of mixture reactivity.

The shadow photographs resolved in some details, the processes of turbulent flame propagation and DDT. Their comparison with the data from the RUT tests showed that not only the critical conditions, but the detailed picture of the processes of the onset of detonations are similar, if geometry is scaled with  $\lambda$ .

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## PROPAGATION, DECAY AND REIGNITION OF DETONATIONS IN TECHNICAL STRUCTURES

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In the present work, an experimentally proven mathematical-physical model for detonative propagation, decay and reignition processes in technical structures is developed. The model enables the analysis and assessment of complex technical structures with respect to safety in case of detonative combustion.

First, on the basis of Zel'dovich – Döring – von Neumann theory, a two-step model for the chemical reaction was developed, considering all the important thermal material properties and their influence on the structure of detonations. In agreement with experiments using a variety of hydrogen, oxygen and inert gas compositions, the relation between the degree of irregularity in detonation cell structure and the heat capacity is analyzed and described:

In mixtures with high heat capacity and therefore low Neumann-shock temperature, strong transverse shocks are necessary to maintain the detonation propagation process. The transverse shock waves lead also to sudden reignition of the already decoupled areas of the detonation front, initiating irregular structures of the detonation front. This means (e.g. for the detonation-to-deflagration processes), the transition can happen only when overcompressed because at that time no transverse shocks are still existent.

For further experimental verification of the developed model, the detonation processes through tubes, with abrupt changes in their cross-section, are investigated. For this purpose, the mechanisms and phenomena of decoupling processes of shock and flame fronts, and the detonative reignition due to shock reflections have been systematically investigated in experiments. As a result, the following mechanisms and phenomena are analyzed and described.

At entry cross sections larger than the critical tube width the maintenance of detonations (at the side already decoupled) takes place by cross-detonations out of the middle of the detonation front. Below

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the critical tube width, shock and flame will decouple completely behind the expansion of the cross section. Due to the Mach reflection of the bowed main shock at the confining walls, a detonative reignition is possible. The quantity of detonation cells necessary for this reignition is often smaller than the value of the critical width. The condition for reignition is the achievement of an overcompressed state at which the detonation can propagate without transverse shock waves. In case of steep cross section increase, there exists an expansion ratio of cross sections, above which detonative reignition is impossible after decoupling of the shock wave and flame. Besides the critical width or diameter, this expansion ratio of tube cross sections is an important parameter for safety assessment of technical structures, in which detonative combustion occurs.

The similarity criterion for scaling the decoupling mechanisms from laboratory to technical dimensions is the ratio of detonation cell size to the cross section at the entrance of the tube. In addition, the propagation Mach numbers are considered for detonative reignition processes. With that, the transferability of lab-scale experimental results to technical scale is possible using simulation calculations with the developed model.

To show the applicability of the experimentally validated model for full scale detonation arrestors, an improved full size design has been developed and tested. In most of the present detonation arrestors, detonative reignition downstream of the arrestor device is a serious problem. The developed innovative design of detonation arrestors is based, both on the expansion of the detonation in an expansion volume inerted by pre-combustion inherently initiated by the detonation itself, and corresponding design measures. By this means a high non-penetrating reliability is ensured.

## INVESTIGATION OF $H_2$ + AIR FAST FLAME PROPAGATION IN TUBE WITH MULTI-DIMENSIONAL ENDPLATES

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A set of experiments in a tube (filled by  $H_2$ +Air mixtures) with partially obstructed area and multi-dimensional endplate was performed. Three main regimes of loading from explosive combustion of  $H_2$  + Air mixtures near the obstructed area can be distinguished on the basis of tests performed.

First Regime: At  $H_2$  concentration in mixture with air exceeding 20% vol., a non-decaying quasi-steady complex (QC) is emitted from the obstructed part of tube. QC consists of the pressure wave (SW) followed by the combustion zone ( $FF_1$ ). The speeds of SW and  $FF_1$  are close to each other. The reflection of QC at the end wall generates a reflected pressure wave in combustion products and that process does not depend on the reflector type.

Second Regime: At  $H_2$  concentration, ranging from 15 to 20% vol., a decaying complex SW – decelerating flame front ( $FF_2$ ) is emitted from the section with obstructions. Reflection of SW results in a reflected shock moving in unburned precompressed mixture ahead of  $FF_2$ . The reflection at the flat endplate is not accompanied by additional self-ignition phenomena. Concave reflector gives rise to secondary explosion waves arising from hot exothermic centers inside the non-flat reflector.

Third Regime: At  $H_2$  concentration below 11% vol., the speed of propagating flame inside obstructed zone is sufficient only to generate a set of acoustic waves ahead of decelerating flame. Reflection of these waves, irrespective of the type of reflectors, does not lead to a significant effect on overall pressure increase during combustion in the tube.

## DETONATION IN GASEOUS REACTIVE MIXTURES AT HIGH INITIAL TEMPERATURE

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Up to now the initial temperature effect on detonation phenomena has not been widely studied. Since there is a great need to assess possible explosion hazards, it is important to know the influence of this parameter.

To perform such a study, experiments were conducted in a detonation tube (53 mm inner diameter, 7.2 m long) made of 304 L stainless steel. This tube is supplied with a low voltage, high intensity electrical power source (18.6 V-DC, 1700 A) and heated by the Joule effect to a temperature as high as 900 K at a rate of about 100 K per minute. The temperature variation along the main part of the tube (about 6 m) is less than 5 K at 600 K. A shorter detonation tube, of variable length between 10 and 50 cm, is connected to the previous one and filled up with a very reactive gaseous mixture so that its detonation induces a shock-to-detonation transition in the heated mixture (both mixtures are separated by a mylar foil).

Detonation velocity is measured all along its propagation using a hyper-frequency Doppler interferometer. Detonation cellular structure is recovered using the classical smoked foil technique.

In order to assess the initial gaseous mixtures composition at high temperature, chromatography analysis of samples have been made with respect to temperature, pressure and stay duration in the heated detonation tube. Such analysis allowed to determine the maximum initial temperature that each mixture can support without a considerable evolution in composition.

Stoichiometric  $C_nH_m-O_2$  mixtures diluted with 50% Ar at a maximum initial temperature  $T_0$  of 600 K (according to the mixtures) and in the range of initial pressure  $P_0 = 0.1-1$  bar were studied.

The experimental results show two main trends in the behavior of the detonation cell size  $\lambda$  with respect to  $T_0$ , so that gaseous explosive mixtures can be classified into two groups depending on the value

of their reduced activation energy ( $E_a/RT$ ) in the Zel'dovich - von Neumann - Döring conditions:

$$\begin{aligned} \text{For } E_a/RT \leq 5 \quad \lambda &\propto P_0^{-n} T_0^m \\ \text{so that} \quad \lambda &\propto \rho_0^{-n} \quad \text{with } n \sim 1.2 \\ &\quad (\rho_0 \text{ is the initial density}) \end{aligned}$$

$$\text{For } E_a/RT \geq 5 \quad \lambda \propto P_0^{-n} T \quad \text{with } 1.2 < n \leq 1.3$$

So, in the latter case  $\lambda$  is independent of  $T_0$  and therefore of the initial density for a given initial pressure.

## SOME ESTIMATIONS OF THE POSSIBILITY TO REALIZE SHOCK-INDUCED COMBUSTION

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The use of detonation combustion in scramjets and ram accelerators has been widely discussed recently. A system of mathematical models, numerical methods, and computer codes based on numerical solution of parabolized or full Navier-Stokes equations for viscous reacting flows was developed in CIAM. This system allows to simulate the shock-induced combustion using detailed schemes of chemical reactions, taking into account turbulent mixing of fuel, supplied separately, and air and boundary layers on the duct walls. Adaptive grids are used to increase the computational accuracy.

Some model problems are considered to estimate the influence of realistic factors (finite rates of chemical reactions, non-uniform composition of combustible mixture in front of the shock, and the existence of boundary layer on walls) on the possibility of detonative combustion.

The first problem considers the hydrogen-air premixed flow in a 2D model combustor with inflected upper wall. The oblique shock is generated at the point of contour inflection. This shock can be used for flame ignition and stabilization. The influence of temperature and composition of combustible mixture, as well as the angle of the wall contour inflection on the flow structure was investigated. The main attention was focused on the interaction of the chemical reaction zone with the shock and on the detonation structure arising as a result of this interaction. Different detonation structures, which include the detonation shock, are observed depending on free stream conditions. Processing and analysis of the computational data revealed some flow features during formation of the detonation structure. Primary attention is paid to the conditions governing the detonation structure. Transition from steady to unsteady flow regimes is also considered and the conditions are analyzed at which this transition occurs.

The second problem deals with investigating the possibility of realization of a scramjet with detonation combustion induced by a shock, generated by the leading edge of the inlet cowl, when the fuel is supplied upstream of the engine entrance. The mixing process upstream the engine entry is considered when hydrogen is injected in the forebody region. A possibility of realistic non-uniform mixture ignition by the shock is estimated. The influence of the forebody boundary layer on mixing and on premature ignition in front of the engine entrance is analyzed. Main features of combustion in the duct behind the shock are analyzed, taking into account finite rates of chemical reactions, mixing, and wall boundary layer.

The third example is concerned with the investigation of detonation combustion in a duct of ram accelerator at different projectile Mach numbers. The variation of the flow structure with the Mach number is analyzed using a detailed scheme of chemical reactions and a high resolution finite difference scheme.

## EFFECTS OF COMBUSTION-GENERATED WAVES ON THE REYNOLDS STRESS BUDGET

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Pressure waves are generated in supersonic combustion due to the strong coupling between compressibility and chemical heat release. Such a wave is expected to change the flow along its path, and the modified flow will in turn affect the combustion process. Until very recently, the interactions between flow and combustion were considered in a global manner, that is, only mean quantities were studied, even though the flow is usually turbulent, as in the case of detonation. The new technique of Direct Numerical Simulation (DNS) marks a new era in the study of turbulence-combustion interactions. Because DNS solves the original governing equations without modeling, the solution contains full information about the turbulence and combustion over the whole spectra of time and length scales. This enables detailed investigation of unsolved fundamental problems, such as wave effects in reacting turbulent flows. Recently, Luo and Bray [1] examined the combustion-induced wave effects on turbulence generation, conserved scalar and stagnation enthalpy transport, using DNS of turbulent diffusion flames. Among the findings of importance are (1) the strong pressure wave effects on combustion-generated turbulence and (2) the existence of local counter-gradient diffusion (CGD) of a conserved scalar flux when the heat release was strong.

The present paper examines the combustion-generated wave effects on the Reynolds stress budget. The terms in the transport equations of  $\rho u_i'' u_j''$  are computed using DNS databases of turbulent diffusion flames. The DNS solved the full time-dependent compressible Navier-Stokes equations coupled with a one-step chemical reaction governed by the Arrhenius kinetics. The reacting flow has a convective Mach number of 1.2. Various heat release rates are simulated. The wave effects are seen to increase with increasing heat release. The wave effects influence the Reynolds stress budget through the combustion-induced pressure fluctuations. Direct wave effects are thus reflected

in the pressure-strain and the pressure-velocity correlation terms. However, combustion-induced density and temperature fluctuations affect the production, dissipation and diffusion terms. All these effects are analyzed in comparison with the non-reacting case of the DNS databases. The final paper will also look at the modeling issues involved. Another important area to examine is the link between acoustics and combustion waves.

The above simulation conditions are undoubtedly far from those found in detonation. Despite tremendous progress in supercomputing techniques in recent years, DNS of detonation waves in turbulence is still out of reach. However, the underlying physics of turbulence-combustion interactions in supersonic flow is believed to be similar. The present study is just one step towards understanding the complex phenomenon of combustion waves in the turbulent compressible media. One objective of this paper is to increase the cross-fertilization among the previously separated subjects of detonation and turbulent combustion.

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## NUMERICAL MODELING OF FLAME ACCELERATION TO DETONATION IN GASES

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Reliable quantitative ab initio models simulating deflagration-to-detonation transition (DDT) are still very far from their complete development, although qualitatively there are no problems in understanding the main features of the process. One of the most interesting peculiarities which is extremely difficult to treat is the so-called hot spot ignition and run-away of the reaction wave to a self-sustaining reactive shock near these hot spots. Therefore a realistic model must incorporate the processes responsible for both hot spot formation and the growth of a perturbation generated by this hot spot to a detonation-like wave. Both these problems call for thorough investigations which present difficulties, because of the necessity of including into a model a great number of physical processes whose mathematical treatment requires quite different approaches. These processes are propagation of curved laminar flames, flow turbulization, interaction of oblique shock waves with each other and with flame zones, and self-ignition. Whereas generation of self-sustaining reactive shock waves in temperature and concentration fields with gradients was a subject of many investigations (see, e.g., [1, 2]), the problem of hot spot formation in DDT processes was never tackled seriously. Only recently, the availability of sufficiently powerful computers made it possible numerical solution of the equations governing these processes, at least under some physically reasonable simplifying assumptions.

This work is an attempt to numerically model detonation initiation in the flow field produced by the accelerating flame in a duct. The main attention concentrated on exploring the feasibility of hot spot formation. Hot spots capable of generating self-sustaining reactive shock waves are produced, either due to flow fluctuations which may inject small volumes of combustion products into the unburnt mixture (and vice versa) and increase thereby the rate of heat release, or due to collisions of oblique shock waves arising ahead of the flame front.

In this work, the second process is assumed to be dominant. The problem was solved numerically in a 2D plane geometry with allowance for turbulence which was described by a slightly modified  $k-\epsilon$  model [3]. Shock discontinuities are captured using the second order Godunov method. Both laminar and turbulent flame fronts were also captured with the aid of the method suggested in [4]. Calculations yielded a full space-time pattern of flow development from a laminar flame to turbulent burning with formation of large-scale 'tongues' and a set of 2D shock waves interacting with each other and with the flame. The flow field shows hot spots at the sites of shock wave collisions in which intense reaction starts. The reaction kinetics is approximated by a global Arrhenius equation derived from experiments on self-ignition behind shock waves.

In spite of the adopted simplifying assumptions, the calculation results are consistent with available data on the pre-detonation distance.

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## ON THE INTERACTION OF GASEOUS DEFLAGRATION AND DETONATION WAVES WITH OBSTRUCTIONS

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Estimations of the mechanical effect of deflagration and detonation waves on obstructions or structures are based, as a rule, on the parameters of stationary propagating regimes. However, the combustion regimes with overshooting values of the parameters are also reported [1, 2]. The latter is caused by the essential dependence of combustion processes, which govern spatial and temporal scales of energy deposition, on the thermodynamic parameters of environment. In the present work, the numerical simulation of interaction of incident deflagration and detonation waves with obstructions was performed on the basis of a kinetic scheme consisting of nine chemical reactions. The analysis of results shows that subsonic deflagrations exhibit non-monotonic dependence of the pressure at obstruction walls on the intensity of the incident wave. If the initiation energy is insufficient for generation of a steady detonation wave but reasonably close to the critical value, the pressure in the reflected deflagration wave can essentially exceed the value relevant to the reflected detonation wave. The range of initiation energies, which result in reflected pressure values exceeding the pressure in reflected detonations by several times, is rather narrow and corresponds to the range of transient combustion regimes.

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## SHOCK AND DETONATION WAVES INTERACTION WITH ENTROPY LAYERS

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Shock wave interaction with the longitudinal entropy layer leads to the flow reorganization with two possible outcomes [1]: either the establishment of the regime with the new stationary configuration of a shock front and its propagation at a constant velocity, or the appearance of the non-stationary regime with vortex formation behind the shock front and continuous flow reorganization with the shock propagation along the entropy layer.

The aim of the present work is numerical modeling of interaction of shock and detonation waves with entropy layers, and the analysis of the arising flow regimes. It was shown that the criterion for transition from one above mentioned regime to another requires the two following conditions to be satisfied: (1) static pressure behind a detonation wave, propagating through the entropy layer, is equal to the static pressure in main stream behind the main detonation front; (2) the gas velocity behind the detonation wave, propagating through the entropy layer, is equal to the velocity of the main detonation front. It was shown, that the flow development depends on the length of the non-equilibrium reaction zone.

In the present work, two-dimensional numerical simulation of the shock wave - entropy layer interaction is based on the Random Choice Method (RCM) [2]. It is especially important for the analysis of unsteady shock wave interactions that RCM exhibits almost vanishing artificial viscosity and diffusion. A chemical mechanism was approximated by the single-step reaction.

Calculations for different mixtures and different regimes have been performed. The results of calculations and analytical estimations were completely confirmed by the results of experiments [3] for the free detonation wave interaction with a hot layer in  $0.1\text{O}_2 + 0.2\text{H}_2 + 0.7\text{Xe}$  mixture.

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## THE INITIATION OF DETONATION IN A SUPERSONIC FLOW BEHIND SHOCK WAVE UNDER NON-EQUILIBRIUM EXCITATION OF VIBRATIONAL DEGREES OF FREEDOM OF MOLECULES

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Numerous studies have been devoted to dynamics of detonation combustion of various mixtures behind shock waves. However, all these studies assumed that delayed excitation of molecular vibrations behind a shock wave and vibrational excitation of molecules during chemical reactions have no effect on the principal characteristics of the process. It was demonstrated only recently that, in a number of practically important cases, the delayed excitation of molecular vibrations of  $H_2$  and  $O_2$  under detonation combustion of  $H_2$ - $O_2$  mixtures may noticeably influence the induction and combustion zone lengths.

In this report, the results of detailed analysis of the mentioned effects and the influence of preliminary vibrational excitation of molecules on initiation and dynamics of detonation combustion behind a stationary shock wave in  $H_2$ -air mixtures are presented.

A distinctive feature of detonation combustion behind a shock wave, in comparison with combustion in a closed reactor, is that the heat transition into translational degrees of freedom, caused by vibrational relaxation or chemical transformations, occurs in a moving gas and therefore results in a more significant change in temperature and density. This fact together with the change in rate constants caused by non-equilibrium excitation of molecular vibrations leads to the essential change in the detonation combustion rate. Analysis was made on the effect of delayed excitation of molecular vibrations on the dynamics of detonation combustion under supersonic and subsonic flow of reacting mixture behind a shock wave. It was shown that these processes decrease the combustion rate for supersonic flow behind a shock wave, and promote combustion processes for subsonic flow, in comparison

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with calculations using the commonly applied models in which the non-equilibrium excitation of molecular vibrations are ignored. Neglection of delayed excitation of molecular vibrations may lead to significant errors (up to 60%) in induction and combustion zone lengths.

Analysis was made on the mechanisms of combustion initiation under vibrational pre-excitation of  $H_2$  and  $N_2$  molecules in front of a shock wave. Preliminary excitation of both  $H_2$  and  $N_2$  molecules was shown to result in significant intensification of combustion, and reduction of induction and combustion zone lengths (up to 10 times). The composition of combustion products also exhibits changes in this case. The obtained results imply a possibility of controlling detonation processes by the selective excitation of vibrational degrees of freedom of molecules.

## BOILING WAVES OF DETONATION AND DEFLAGRATION TYPE ARISING UNDER ABRUPT DEPRESSURIZATION OF HEAT EXCHANGING CONTOURS

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Investigations of deflagration, detonation and transient processes in chemically active mixtures resulted in the development of a theory of self-sustaining waves propagating in metastable media.

Metastable media can be also represented by systems other than those of chemically active type. It was recently discovered that, under abrupt depressurization of a heated fluid below the saturation level, the superheated fluid in the pipeline preserves its metastable state for a relatively long time. Intense boiling begins only after arrival of a slow rarefaction wave (travelling at velocities about 10 m/s). The existing theories of equilibrium and non-equilibrium boiling fail to explain the phenomenon.

This paper presents a model of self-sustaining boiling waves propagating in superheated metastable fluids. The model takes into account bubble formation, growth, and breakup in accelerating non-equilibrium two-phase flows.

Once fluid is depressurized, a fast rarefaction wave propagates in a duct from an open end at velocities about 1000 m/s. This wave drops the pressure below the saturation line and brings fluid to a superheated metastable state. Boiling starts on a limited number of boiling centers, present in fluid, since bubble size has to exceed a certain characteristic size in order to grow rather than to collapse due to surface tension. The expansion of a fluid-vapour mixture brings to its efflux from the open end of the duct. The difference between accelerations of bubbles and fluid in a two-phase flow results in an increase in their velocity difference, and that turns out to be sufficient to cause breakup of growing bubbles due to interface instability. Thus, the fluid-vapour interface increases, and boiling intensifies. The boiling intensification causes further acceleration of the fluid-vapour mixture

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and increases the difference in velocities resulting in further breakup of bubbles. Thus, mechanical non-equilibrium in two-phase mixtures creates the conditions for a chain process of bubbles breakup in slow rarefaction waves propagating in two-phase media, wherein one breakup event provides the conditions for successive breakup events. This rapid process of evaporation intensification takes place in a narrow zone, where fluid and vapor are brought to a state of thermal equilibrium.

Physical and mathematical models, developed in this paper, describe very well the existing experiments on propagation of slow boiling waves in superheated fluids and explain the mechanism of the process.

Numerical modeling of fluid boiling under its depressurization was undertaken for different sets of initial conditions. The central thin layer of fluid was assumed to be heated 10 K higher than the rest of fluid. The results show that, when entering the heated zone, the slow boiling wave initiates a more intensive boiling and pressure raise in the zone, resulting in two compression waves propagating in both directions, similar to 'detonation' and 'retonation' in chemically active media. The 'detonation' wave propagates at supersonic velocity of 200 m/s (the speed of sound for a specified multi-phase mixture is 26 m/s). It initiates rapid breakup of bubbles and brings the mixture to an equilibrium state at the elevated pressure. The 'retonation' wave degenerates rapidly after entering the equilibrium mixture. Thus, the process has very much in common with deflagration-to-detonation transition in chemically active media.

## BUBBLE DETONATION AND ITS PROPAGATION LIMITS

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Detonation waves were studied experimentally in different bubble media:

- mono-component systems: (I) non-reactive liquid - bubbles of the mixture of reactive and unreactive gases, (II) liquid fuel - bubbles of the mixture of gaseous oxidant and unreactive gases;
- multi-component systems: (I) non-reactive liquid - association of reactive and non-reactive gas bubbles, (II) liquid fuel - association of gaseous oxidant and non-reactive gas bubbles, (I-II) liquid fuel - association of gaseous oxidant and reactive gas bubbles;
- polydisperse systems: (I) non-reactive liquid - reactive gas bubbles of various size.

The occurrence of a detonation wave is possible if the energy loss in the wave is compensated for by the chemical energy released in the wave. In this case, the relation between the chemical energy inherent in the medium and its dissipation in a tile detonation wave (energy balance) rather than the absolute energy content in the medium (it is least in bubble systems) is important.

If the energy content of the medium is lower than a certain value or the energy loss in the detonation wave is higher than a critical value, the occurrence of a detonation wave is impossible. Such factors as (1) the dilution of a reactive gaseous mixture in bubbles with an inert gas (mono-component systems), (2) the presence of non-reactive bubbles in the system among other reactive gas bubbles (multi-component ones), or (3) the existence of bubbles of various size in the liquid, reduce the energy content of the medium and increase the energy loss of the detonation wave. Hence, the domain of existence of detonation waves in bubble media may be affected by many factors.

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Some detonation limits (lower and upper) have been found experimentally in terms of gas phase concentration in the system, the content of gaseous mixture in bubbles, and the bubble diameter. The lower limit of detonation waves in terms of the viscosity of liquid component is found. Some energy related limits of detonation waves are found and their domains of existence in mono- and multi-component bubble media are correlated. The propagation limits of detonation in polydisperse bubble media are also set.

## THE THEORY OF DETONATION STRUCTURE NEAR THE LIMITS OF PROPAGATION

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A closed theory of the marginal stationary detonation regime is suggested based on both the local application of the conservation laws to wave elements of detonation structure and to the whole propagation process. A main element of energy deposition in a limiting (spinning) regime, that is a transverse detonation wave, is considered with due regard for the finite rate chemical kinetics. Additional energy deposition in an oblique wave at the apex of the front is also taken into account.

Based on calculations of detonation structure, the criterion of detonation limits is proposed. It is a requirement of simultaneous implementation of two conditions, which consist in limitation of reaction zone lengths behind the first shock front and behind the front of transverse detonation wave.

Mathematically, the procedure includes integration of chemical kinetics equations. The statement of the problem is reduced to a set of nine algebraic equations, which are integrated by an approximate method. The theory allows for determining the limits of stationary detonation regimes.

## ON DETONATION CONTROL IN DUCTS BY ELECTRIC DISCHARGES

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Deflagration-to-detonation transition is known to involve a number of stages such as ignition, pre-detonation and detonation onset. The pre-detonation stage is characterized by formation of developed turbulence, increase in the speed of wave processes, and acceleration of flame. As is shown in [1, 2], electric discharges affecting the flame zone due to intrinsic feedback allow the unstable combustion wave to be controlled. A current-stabilized discharge will suppress the combustion instabilities and stabilize the combustion wave, whereas a voltage-stabilized discharge, by contrast, will enhance those instabilities. In the case of detonation, it allows the transient processes to be controlled. The paper presents the results indicating that in ducts, whose walls form a discharge chamber, the time required for a combustion process to transit to detonation generally increases when a current-stabilized discharge is applied, while in the case of a voltage-stabilized discharge that time will be appreciably reduced. To summarize the above, the results discussed illustrate that electric discharges enable detonation initiation to be controlled.

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**APPLICATIONS  
OF  
DETONATION  
PHENOMENA**

## EFFECT OF NOZZLE GEOMETRY AND SIZE ON THE PROPULSIVE PERFORMANCES OF DETONATION

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Presented are the recent developments on the effects of nozzle size and geometry on the propulsive performances of a detonating charge contained in a cylindrical chamber. The framework of the study is propulsion by means of the Pulsed Detonation Engine (PDE). The previous engine configuration [1] consisted of a cylindrical combustion chamber (CC) with one end, called the thrust wall (TW), closed. During an operation cycle, the CC was completely filled with the reactive charge and the detonation products were released directly to the atmosphere via the open-end of CC. In this case, the emerging shock wave is fairly strong and the rarefaction wave, that backs up from the open end of CC to TW, induces a quick decay of the overpressure in CC, and then on TW. Future design modifications may be required to set up a nozzle, in order to slow down the decrease in the overpressure on TW, by attenuating the shock wave in the nozzle before its transmission to the atmosphere. This results in an augmentation of the specific impulse and in an attenuation of the shock wave in the immediate vicinity of the engine. In the present work, straight and diverging nozzles are added at the end of CC and the effect of the ratio  $\alpha = l/L$  ( $0 < \alpha \leq 1$ ,  $l$  is the CC length,  $L$  is the total length of device, including nozzle) on the propulsive efficiency is determined via the TW detonation pressure histories and ballistic pendulum method. The specific impulse  $I_{sp}$  and the characteristic time of a single cycle are expressed as functions of the Chapman-Jouguet characteristics of the reactive charge and of the scale of the geometrical configuration. As  $\alpha$  decreases from 1,  $I_{sp}$  increases but the application time of the thrust on TW also increases, which limits the potential operating frequency of the PDE. The optimal operating configuration is then discussed in terms of the specific impulse and of the maximum operating frequency.

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## THEORETICAL AND EXPERIMENTAL MODELING OF DETONATION PULSE ENGINE

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**Electrochemical Pulse Jet.** The development of new types of internal combustion engines is of significant interest both for theoreticians and experimentalists. A relatively new scheme referred to as the electrochemical pulse jet has been studied by S. Wojcicki. An electrical discharge (intense spark) in the combustion chamber is used to improve efficiency of conversion of thermal energy into mechanical energy by increasing the engine compression ratio. This electrical discharge, which is much more intense than that used in conventional internal combustion engines, can convert combustion into detonation and explosion. The electrical discharge arises in the combustion chamber when the flame front impinges on special electrodes that are attached to a pre-charged energy storage capacitor. Electrodes with the Rogowski profile eliminate electric field enhancement near the electrode edges. A 'collar' (ring-type) discharge creates converging shock waves in the combustible mixture, leading to a fast burning process with detonation, high pressure, and an increase in the compression ratio. The energy of combustion in a single cycle is much higher than the electrical energy delivered by the electrical discharge.

**Simulation and Experiments.** Modeling of these processes includes the converging shock and detonation waves and the energy input from the discharge. Numerical simulation of gas flow in the chamber and in connecting intake and exhaust tubes has been implemented by applying quasi-one-dimensional and two-dimensional approaches. Chemical kinetics, wall friction, and heat losses are included into the model. In this paper, the results of calculations are reported for several

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sets of initial conditions and types of combustible mixtures. The output of the model includes impulse and thrust values as well as engine efficiency.

A small-scale experimental setup was constructed and preliminary data was obtained. The setup will be modified and used to create intense spark channels which will initiate the implosion in the combustion chamber.

Preliminary results have been reported in [1-5].

**Future work.** Appropriate comparisons between experiment and theory will be made. The work will result in a detailed model of this new type of engine. The model can be used to design large scale jet engines for hypersonic passenger airplanes, to improve operation in high speed regimes and for underwater small submarines.

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## MHD POWER GENERATION FROM A PULSE DETONATION ENGINE

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The problem of electrical power extraction from a Pulse Detonation Engine (PDE) is addressed through preliminary numerical investigations of the efficiency of a Magneto Hydro-Dynamic (MHD) generator coupled to a generic PDE. The MHD generator does not obstruct the flow in a PDE, and has the potential for high performance, given the combination of high temperature and high velocity flow of the detonation wave and of the blow down process immediately following it. A generic PDE-MHD device is selected and modeled as a planar (2D) configuration, consisting of a tube of constant cross-section and a nozzle. Single pulse CFD calculations are performed for various cases of design parameters, and using a simple model of the MHD interaction. The electric and magnetic fields are assumed constant and uniform within a certain region. Variations of the extracted electrical energy as a function of nozzle expansion, interaction length, magnetic field strength and thermo-chemistry are studied. Calculations are performed for the case when a single continuous electrode is used with the applied voltage automatically adjusted for maximal power, and compared to the ideal case of constant loading at each point within the flow. It is found that there is an optimal nozzle expansion ratio, and an optimal interaction length. The latter is a result of the large flow variations within the entire tube. Absolute optimization of the power can be achieved only for different values of the voltage at different locations. For a single electrode, it is shown also that the performance does not scale as the square of the magnetic field, as would be expected from the ideal, constant-loading approximation. This scaling loss has an important consequence on the design of the generator, since it indicates that the system is not efficient at high field strength. It is possible, however, to recover the scaling and increase the performance by using multiple electrodes. It is also shown that the power extraction has a negligible effect on the thrust produced. The calculations also show a strong sensitivity to the thermo-chemical variations, notably to the values of elastic electron-impact cross-sections. Realistic extrapolations of the numerical results indicate that power levels of 100 kW could be achieved with off-the shelf technology. Higher power levels can readily be achieved with different designs of the PDE-MHD system.

## COMPUTATIONAL AND EXPERIMENTAL INVESTIGATIONS OF THE PULSE DETONATION ENGINE

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Creation of new types of aviation engines that utilize more completely the chemical energy of fuel is an important current problem of modern mechanical engineering. Arranging two-stage combustion in a pulse detonation regime is one of the possible methods for producing thrust. Presented in this report are the results of computational and experimental modeling of the pulse detonation engine with the ring nozzle arrangement and a half closed spherical cavity afterbody.

The conditions for arising the pulse air flow and the thrust as a function of pressure and geometrical parameters of the nozzle were determined experimentally. It is found theoretically that the products of the first combustion stage are able to support exothermic reactions resulting in various combustion regimes including detonation. The computational results on gas composition in the two-stage combustion of acetylene in air and the estimations of increasing the specific impulse are presented. Also reported are the experimental investigations of the flow of acetylene-air combustion products through the axially symmetrical nozzle arrangement with a half closed cavity. Estimations of the specific impulse shed light on the efficiency of such arrangements for producing thrust.

## RAM ACCELERATORS IN THE DETONATIVE MODE

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In principle, the ram accelerator is a propulsion concept in which oblique detonations can be effectively used to attain much higher velocities than with other combustion mechanisms. In the ram accelerator, a projectile that resembles the center body of a ramjet travels at supersonic speeds through a premixed fuel-oxidizer mixture enclosed in a tube.

Several combustion mechanisms are possible, depending on the velocity of the projectile and the composition of the mixture in the ram accelerator. Since the projectile travels at supersonic speeds, oblique shocks are formed at the nose of the projectile and they subsequently reflect from the side walls of the tube and the projectile body. Depending on the strength of these oblique shocks, ignition may occur after the initial shock or subsequent reflections. Energy release may couple with the shock wave to form oblique detonations. In order to maximize performance, the oblique detonation must be generated and stabilized at appropriate locations in the system. Therefore, successful development of such systems depends on the knowledge of the structure and stability of these detonation waves and understanding the related transient physical and chemical processes.

Extensive computational and experimental studies have been carried out on the ram accelerator in the detonative mode. Some of these studies have focused on the detailed structure and stability of detonation waves while others have investigated the effect of material and gas composition on the overall performance.

In this paper, an overview of many of these studies are presented with an emphasis on the transient dynamics of the detonation structure on an accelerating projectile. For example, detailed numerical simulations show that as the projectile accelerates, the detonation moves from one shock to the one ahead of it, because of the strengthening of the shocks and the consequent reduction in induction times. Ultimately,

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the detonation would occur behind the first oblique shock and produce no positive thrust. That is, there is a maximum velocity that can be achieved for any given mixture with a specific projectile. The effect of such gas-dynamic limits and other limitations due to material properties of the projectiles used in the experiments on the further development of the ram accelerator are discussed.

## **USE OF ELECTRO-PHYSICAL PROPERTIES OF DETONATION PRODUCTS IN THE EXPLOSIVE FAST OPENING SWITCHES**

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Realisation of academician A. D. Sakharov's concept of magnetic cumulation has allowed at the present time to create an explosive magnetic generator (EMG) with a stored energy up to  $10^8$  J. However, if some special measures are not undertaken, the EMGs cannot form a current pulse of microsecond duration. Utilization of the effect of current contour rupture by means of explosive fast opening switches helps to perform fast energy supply from the EMG to the load. The rate of energy supply from the EMG to the load depends on the electro-physical properties of detonation products of the explosive charge. The use of electro-physical properties of detonation products in the explosive fast opening switches is considered in the report.

## NUMERICAL INVESTIGATION OF FLOWS WITH SUPERSONIC COMBUSTION IN UNDERDRIVEN AND OVERDRIVEN DETONATION WAVES

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This paper summarizes the results of a series of numerical simulations implemented in 1995–1998 of gas dynamics of flows with supersonic combustion. Simulation of inviscid flows with hydrogen–air combustion was performed by the second order numerical method. The method is based on the explicit Godunov–Kolgan–Rodionov scheme for the description of convection and on the point-implicit approach to the approximation of chemical sources. Stationary flows were calculated using the time-marching approach.

All the investigations dealt with oblique detonation waves. The analysis of fine spatial structure of detonation fronts is presented in a number of computational [1] and experimental [2, 3] studies. Nevertheless, the Zel'dovich – von Neiman – Döring (ZND) model [4] still remains efficient for the analysis of integral flow characteristics behind oblique detonation waves. The primary purpose of the computations described in this paper was to investigate the influence of finite-rate chemical reactions on the flow structure without regard for the inner structure of detonation fronts. In all the computations, the cells of a computational grid were sufficiently smaller than the induction length in the main part of computational domain; however they were of the order of detonation front thickness. As a result, the detonation waves were actually considered in the framework of ZND-model. Physical processes in the rest of flowfield (i.e. processes associated with generation and stabilization of detonation) were simulated with non-equilibrium reactions taken into account.

The following problems were addressed:

- (1) What type of structure is generated near the wedge surface in the flow of non-equilibrium reacting mixture?

- (2) Is it possible to stabilize combustion in a detonation wave by decreasing the wedge angle?
- (3) How the flow structure about the 'wedge-flat body' configuration depends upon the length/height of the wedge? What will happen when the wedge length tends to zero, and the body degenerates to a flat plate?
- (4) How the flow structure with the oblique detonation wave varies with the increase in the wedge angle?
- (5) What is the similarity and difference between the flows of detonating mixture near the wedge and about the cone?
- (6) Is it possible to arrange the stationary combustion in fully inviscid, non-equilibrium flow in such a way that the gas velocity in any point of the flow would exceed the speed of sound?

The results described in this work are of interest for the theoretical developments and for the utilization of operational process in combustion chambers of realistic technical devices.

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## ON THE FORMATION OF DUSTY GAS DETONATION PROCESS IN COAL MINES

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Investigation of unsteady processes behind shock waves propagating in a gas-particle combustible mixture is important for understanding the mechanisms of industrial dust explosions, such as those in coal mines, which often cause disaster. Presented in this paper are two aspects of the problem.

The first aspect concerns the questions related to ignition and burning of the mixture behind strong shock waves. The results are given on numerical simulation of transition to detonation and on 2D structure of unsteady detonation in the mixture of coal particles with air. The moving medium in the model is considered as a two-phase, double-velocity and double-temperature continuum with mechanical and thermal interaction between phases, and with devolatilization (extraction of volatiles from particles), homogeneous and heterogeneous exothermic chemical reactions, and radiation heat conduction taken into account.

The second aspect concerns the problem of dust entrainment from the layer and dispersion behind a shock wave. It is well known that the pressure wave, e.g. the wave induced by burning gas in a coal mine, disperses coal particles from the walls of a mine gallery into the gas stream and forms an explosive dust cloud. As a result, the initial explosion can become self-sustained and propagate large distances. Despite this problem being investigated by many researchers, there is no complete understanding so far about the mechanism mostly responsible for intensive lift of the particles from the layer. This paper attempts to simulate the particle lift and dispersion by taking into account lifting forces due to particle rotation (Magnus force) and gas-phase vorticity (Saffman force). It is shown that these forces can essentially affect the flow pattern behind a shock wave, resulting in explosive-like dust entrainment and dispersion from the dust layer.

**APPLICATION OF A DOUBLE  
NON-STATIONARY DISCONTINUITY  
REGIME FOR SURFACE DEPOSING  
OF  $\text{Al}_2\text{O}_3$  ENRICHED WITH THE  $\alpha$ -PHASE**

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Described is the construction of the detonation combustion chamber (DCC) supplied with a device of additional ignition, permitting to realize a detonation in a double non-stationary discontinuity regime (RDND) with a probability of 0.995. The DCC working in RDND was used for the deposition of aluminium oxide (ChDA brand, granulation 40–50 and 50–63  $\mu\text{m}$ ) on a steel support. The flow rate of methane–oxygen mixture, pulse repetition rate and spraying distance were maintained constant during the deposition process. The obtained coverings have a high content of  $\alpha$ -phase (up to 70%). The increase of  $\alpha$ -phase content in  $\text{Al}_2\text{O}_3$  coverings is known to result in the increase of its thermal resistance. Thus, the use of RDND allows to create protective coatings based on  $\text{Al}_2\text{O}_3$  with the increased content of  $\alpha$ -phase and the strength of sticking with the steel support not less than 16 MPa, that leads to the increase of thermal resistance of protective coatings.

## DETECTION OF HYDROGEN-AIR FLAMES BY AN ADVANCED PHOTODIODE PROBE TECHNIQUE

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Both laboratory and large scale simulation of accidental hydrogen-air explosions require the development of proper measuring techniques for detecting flames (detonations). The commonly used non-contact experimental procedure is based on the observation of flame front through multiple optical ports. The use of photodiodes as sensitive elements in such a configuration shows some restrictions in the accuracy of measuring the flame position. This is caused by the presence of scattered light emitted by burning products prior to the arrival of a flame front to the point of measurement.

The present work describes an advanced photodiode probe technique which allows to separate the scattered and direct flame emission when applied to propagation of hydrogen-air flames in ducts.

The method is based on the analysis of the near infrared emissivity spectrum of water vapor which presents a main combustion product. The use of photodiodes combined with proper interference filters allows to reveal peculiarities of scattered emission. The spectrum of scattered light was found to be consistent with the black (gray) radiation law while the direct flame front (water vapor) emission appears to be selective. The advantages of the technique for detecting the flame position were demonstrated in the experiments using 50 mm and 120 mm explosion tubes and mixtures with 10-30% hydrogen in air.

## DYNAMIC EFFECTS IN HETEROGENOUS MIXTURES

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Shock-wave compressibility of porous metals has been studied for a range of shock pressures produced by means of detonation waves. There were no experimental data available for this pressure range and for these metals. Measurements were carried out by both the well-known discrete electric pins method and by the newly suggested method of continuous registration of the wave front trajectory. A specimen of porous metal itself serves as a resistance transducer. Its electric resistance behind the shock front is very small and could be neglected. Shock compression of porous metals is described by a model which considers the behavior of air in the pores between the grains of metal.

Sliding detonations of sheet and coaxial cylindrical explosive charges were used as loads for explosion pressing of plane and bar specimens of metal powders. Some properties of pressed details were studied. The experimental data were compared with predictions provided by a model based on the field methods.

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**DETONABILITY  
OF  
ADVANCED  
FUELS**

## STUDY OF DETONATION INITIATION IN UNCONFINED ALUMINUM DUST CLOUDS

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It is now commonly accepted that suspensions of solid reactive particles in air, and even in oxygen, are difficult to detonate. Evidence of detonation propagation has been reported only in a limited number of experimental studies performed in tubes, where it was shown that tube lengths greater than 10 m were necessary for the detonation regime to be reached. Until now there are no definitive proofs of the possibility to initiate self-sustained detonations in unconfined clouds of solid particles. Nevertheless, many two-phase systems of this kind have a specific energetic content comparable (or even greater) to that of 'classical' detonable gaseous mixtures. Hence, it may be presumed that heat release rate is insufficient to support detonation. But the exact reason is not elucidated: is it due to the low reactivity of particles (in connection with their characteristic diameter), or to the formation of low concentration zones behind the leading shock front (caused by the relaxation of solid particles in the gaseous flow) where the composition is out of the detonability limits?

Experiments were performed with aluminum-oxygen suspensions contained in polyethylene balloons of about 0.4 m<sup>3</sup>. A spherical blast wave was generated inside the clouds by exploding a TNT charge of variable mass (up to 150 g). Experiments have been performed with either atomized powder (mean diameter 3.5 and 5  $\mu$ m) or with flakes, at different nominal mass particle concentrations.

Until now, no detonation has been observed to be formed in the cloud. In a limited number of experiments, the velocity of the leading wave approached the Chapman-Jouguet (CJ) value at the end of

propagation in the cloud, but the propagation regime was still non-stationary.

Initiation of two-phase clouds of suspended aluminum particles was studied numerically in configuration corresponding to the above experimental conditions. Comparison was made between initiation by a point energy source and by a real TNT charge of finite dimension. First results obtained for  $3.5\text{ }\mu\text{m}$  particles show that the blast wave generated by the initiator decays rapidly whereas solid particles are ignited in the flow downstream, where equilibrium between particles and gases is not achieved. After about 0.4 m, the reaction rate increases, thus increasing the velocity of the leading front. However, after 1 m of propagation, the leading front velocity is not constant and is also smaller than the CJ velocity. This indicates that clouds of larger dimension (2 m diameter) are required (even with pure oxygen based mixtures) to have the possibility to observe the formation of self-sustained detonations in suspensions of aluminum particles. This necessitates to perform experiments at larger scale than the present laboratory-scale experimental setup.

## STABILITY AND INITIATION OF HETEROGENEOUS DETONATION OF ALUMINUM PARTICLES AEROSUSPENSION

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Non-stationary processes accompanying detonation wave propagation in aluminum particles – oxygen aerosuspension are studied on the basis of the mathematical model of heterogeneous detonation [1] taking into account the differences in phase velocity and temperature. In previous works [2, 3], the existence of stationary solutions of various types (Chapman–Jouguet (CJ), strong, and weak detonation with supersonic final state) was shown. In the present work, the stationary solutions obtained earlier are tested for stability in terms of the problem of detonation wave (DW) propagation supported by a piston. It appears that all stationary regimes including the ‘structurally unstable’ weak regime (the regime with the saddle final point where the relative final velocity is larger than the equilibrium speed of sound and smaller than the frozen one) are stable in the double-velocity double-temperature approximation.

The problem of interaction of DW with an adjacent non-equilibrium rarefaction wave (RW), arising after instantaneous removal of a supporting piston, is solved for all the detonation regimes mentioned. The CJ and weak detonations appeared to be self-sustained, while the strong detonation transforms either to CJ or weak regimes depending on the relaxation times of non-equilibrium processes (similar to the single-velocity approximation [4]). Decomposition of DW to a shock wave and a combustion front with the loss of stability was observed in [4] for the weak regime with an unstable transonic final point. Under conditions of velocity non-equilibrium, the DW structure (shock front, combustion zone, and rarefaction wave) propagates steadily in this regime as well. Interaction of DW and RW in this range of relaxation parameters results in establishing a weak detonation regime with a junction of RW and combustion zone in a transonic point. Then, the resultant structure propagates steadily. Thus, the self-sustained regimes comprise the CJ

regime and all weak regimes, including those with the transonic final point.

The problem of detonation initiation by a shock wave was also studied. It is assumed that the half-space is divided with a diaphragm separating combustion products (at high temperature and pressure) and fresh mixture (at ambient conditions). After removal of the diaphragm, a shock wave propagates in the fresh mixture inducing particle ignition and formation of a combustion front. Calculations indicate that, if the initial temperature and pressure in the combustion products are insufficient to initiate detonation, the combustion front arising at the contact surface is lagging behind the leading shock and weakened by the overtaking RW. At an initial pressure of 100 bar and temperature of 2000 K, the combustion front first propagates behind the shock wave for a certain period of time, then merges with it and, amplifying the DW shock, forms either the CJ or weak DW depending on the values of relaxation parameters.

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## KINETIC MODELING OF HYDROCARBON AUTO-IGNITION FOR CONDITIONS RELEVANT TO PULSE DETONATION ENGINES

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The operability of Pulsed Detonation Engines (PDE) is considerably dependent on the fuel used. Of particular importance is the fuel reactivity within a wide range of operating conditions covering both regular modes (cold start, repeatitive detonation initiation and propagation, cyclic mixture stratification and preheating by hot walls, etc.) and irregular phenomena (initiation failure, pre-ignition, deviation in fuel/air/spark or pre-detonator timing, etc.). Thus, the performance analysis of PDE implies the knowledge of kinetic mechanisms of fuel oxidation.

Currently, heavy liquid hydrocarbon fuels are considered as prospective candidates for practical applications due to their advantages compared to light gaseous compounds. The oxidation mechanisms of heavy hydrocarbon fuels account for thousands elementary reactions and are not suitable for multi-dimensional unsteady performance simulations of various PDE design configurations. Continuing studies of [1–3], this paper presents a semi-empirical oxidation mechanism of a heavy hydrocarbon fuel characterized by the octane number,  $n$ . The fuel is assumed to be a blend of  $(100 - n)\%$   $n$ -heptane and  $n\%$  *iso*-octane. Compared to [1–3], the reaction mechanism was extended to allow computations at low initial pressure and to complete mixture burnout.

Verification of the reaction mechanism has been done by comparing predicted auto-ignition delay times with available data obtained by means of rapid compression machines and shock tube techniques. The experimental conditions close to those attained prior and after shock compression of the reactive mixture in PDE, namely, temperature  $650\text{ K} < T < 1200\text{ K}$ , pressure  $1\text{ bar} < p < 100\text{ bar}$ , equivalence ratio  $0.5 < \Phi < 2.0$ , were examined. Reduced reaction mechanisms were

also developed which approximate with a good accuracy the results of detailed calculations within ignition delay time. The reduced mechanisms are intended to be applied in the multi-dimensional simulation of processes in PDE.

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**UNSTEADY STRUCTURE OF A HYDROGEN  
JET AND THE CONDITIONS OF  
SHOCK-INDUCED IGNITION UNDER ITS  
INJECTION INTO AIR AT HIGH PRESSURE**

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Presented are the experimental results on the structure of a reacting hydrogen jet formed by pulsed injection into a shock tube.

Specific features of the jet flow structure are established using optical diagnostics with a proper temporal resolution. These features are associated with three-dimensionality and with wave properties of the flow. A partial character of combustion is experimentally verified. Jet combustion creates an additional source of mechanical energy which exerts a significant effect on the flow pattern. The influence of jet pressure ratio on the transport properties of the medium is emphasized. The goals of further research are formulated.

## **SUPPRESSION OF DETONATIONS BY EFFECTIVE INHIBITORS**

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New experimental results are described on suppression of detonation of hydrogen-air mixtures at atmospheric and higher pressures by means of gas-phase inhibitors, which are significantly more effective, than halons. The important role of chain mechanism in different modes of gas-phase combustion of hydrogen-containing compounds and other combustible gases is pointed out.

## CONTROL OF PRE-DETONATION EXPLOSION PROCESS IN PROPELLANTS

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Deflagration-to-detonation transition in porous propellants includes two intermediate stages: convective burning (CB) and low-velocity detonation (LVD). The paper summarizes the results of experimental and theoretical studies of stabilization and control of CB and LVD. Quasi-steady modes of CB and LVD in propellants with low porosity (2–10%) are considered. The mechanisms and critical conditions of stabilization are analyzed. The experimental data illustrating specific features of the processes are discussed and the effects of the initial properties of charges are considered. The factors are revealed allowing to control actively the propagation velocity of the processes and the intensity of chemical reactions in the burning zone (within the velocity range from 1 to 200 m/s for CB, and from 1000 to 2000 m/s for LVD). Theoretical models of quasi-steady modes of CB and LVD are developed for explaining the experimental observations. Possible ways of applications of CB and LVD in low-porosity propellants are discussed for increasing the efficiency of propulsion and barrel systems.

## SPIN DETONATION OF EXPLOSIVE DUST LAYER IN VACUUMED TUBES

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The spin detonation mode is known to arise in tubes in the vicinity of propagation limits of detonation. It was also observed in heterogenous systems, where liquid or dispersed solid fuel is deposited on tube walls in the form of a thin layer or suspended in a tube volume with gaseous oxygen or air acting as an oxidizer. In all these cases, the gas phase is the important component of the explosive system, allowing for the propagation of an initiating shock wave, which is the integral part of the detonation complex. However, it has been recently discovered, that detonation also exists in suspensions of explosive particles in vacuum, where the initiating shock is absent. New experiments presented in this paper indicate, that the spin mode can occur in this system as well.

Detonation in evacuated tubes with a thin semi-transparent layer of explosive particles (lead azide, PETN, RDX) on the walls was investigated. The tubes made of polyethylene had internal diameter  $d = 2.3$  mm, while those made of glass had the diameter  $d = 2.7$ – $3.3$  mm. Tube lengths in all the experiments were 0.5–0.6 m. Before the experiment, air was extracted from a tube by a forevacuum pump. Detonation was initiated by an electric spark. The velocity of the arising detonation wave and luminiscence of the reaction zone were registered by the streak-photograph method.

The basic results of the experiments are:

- (1) Spin detonation of a thin layer of powder-like explosives in vacuum tubes, arising without an initiating shock wave, has been observed.
- (2) It is shown, for the first time, that spinning detonation can propagate at a velocity higher than the Chapman-Jouget detonation velocity.

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- (3) The ratio of detonation spin pitch to circumference was found to be close to unity, which is characteristic for gaseous mixtures.
- (4) Contrary to known spin detonation modes, the system under study exhibits a 'tail' from the spin head spreading both backward from the reaction zone and ahead of it (at different angle), and losing gradually the luminiscence from the vacuum side.
- (5) Near the detonation limit (in terms of explosive quantity), at low wave velocities the spinning oscillations in the reaction zone can disappear.

## STRUCTURE OF THE DETONATION WAVE IN A CHANNEL PARTIALLY FILLED WITH THE RDX PARTICLE SUSPENSION

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The process of heterogeneous detonation propagating in a cylindrical channel partially filled with a suspension of high explosive (HE) particles is investigated numerically based on the mathematical model of two-phase, double-velocity medium. Three types of structure of a two-dimensional reaction zone are analyzed.

**Statement of the problem.** A channel of radius  $r_e$  is filled with the gas of density  $\rho_{10}$ . HE particles of diameter  $d_0$  and true density  $\rho_2^0$  are suspended in the channel homogeneously with volume concentration  $\alpha_{20}$ . In the left part of the channel ( $x < 0$ ), the suspension is distributed throughout the whole cross section, and in the right part ( $x > 0$ ) the suspension occupies a cylindrical layer of thickness  $\delta r = r_c - r_0$ , where  $r_0$  is the radius of the internal cavity free of particles. A detonation wave (DW) propagates from left to right along the channel. At time  $t = 0$  the detonation front reaches the coordinate  $x = 0$ . For a given set of thermodynamic properties of phases, it is required to determine detonation dynamics at  $t > 0$  depending on five governing parameters:  $r_c$ ,  $r_0$ ,  $\rho_{10}$ ,  $\rho_{20} = \alpha_{20}\rho_2^0$ , and  $d_0$ .

**Results.** It was shown that for low-density suspensions ( $\alpha_{20} \ll 1$ ) only 4 dimensionless criteria govern the problem:  $K = \rho_{20}d_0\sqrt{q_0}/18\mu_{10}$ ,  $Y_{10} = \rho_{10}/(\rho_{10} + \rho_{20})$ ,  $\eta_c = r_c/x_0$ ,  $L = \Delta r/r_c$ , where  $Y_{10}$  is the initial mass concentration of gas,  $L$  is the reduced thickness of the layer,  $x_0 = d_0^2\rho_2^0\sqrt{q_0}/18\mu_{10}$  is the characteristic length,  $q_0$  is the thermal effect of chemical reactions per unit mass of HE particles,  $\mu_{10}$  is the dynamic viscosity of gas at  $T = 300$  K.

The numerical study is performed with RDX particles as an example. At fixed  $K = 316$ , the parameters  $\eta_c$ ,  $L$ , and  $Y_{10}$  were varied. The structure of reaction zones in DW indicates that the flow in a cylindrical channel is essentially two-dimensional. It was found that there exist the geometrical limits of detonation. These are determined by the critical

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values of layer thickness  $L^*$  and channel radius  $\eta_c^*$ , such that at  $L < L^*$  or  $\eta_c < \eta_c^*$  a non-ideal DW fails to propagate and decays.

Three types of self-sustaining detonation regimes are obtained, characterized by:

- (1) stable flow structure ( $Y_{10} = 0.5$ ;  $r_0/l_{CJ} < 1$ );
- (2) unstable (pulsating) structure ( $Y_{10} = 0.5$ ;  $r_0/l_{CJ} > 1$ );
- (3) a structure with a stable vortex ( $Y_{10} \leq 0.333$ ;  $r_0/l_{CJ} < 1$ , where  $l_{CJ}$  is the reaction zone length of the one-dimensional Chapman-Jouguet wave).

The non-ideal heterogeneous DW of type (1) is the channel wave with the classical flow structure. Analysis of two-dimensional DW structure of type (2) shows that longitudinal velocity pulsations of wave front with period  $\sim 4r_c$  are caused by longitudinal pulsations of gasdynamic parameters in the cylindrical channel. Decrease in initial gas pressure (decreasing  $Y_{10}$ ) results in transition to detonation regimes of type (3). At  $Y_{10} \leq 0.333$ , the heterogeneous DW was found to propagate in an underdriven mode, and a stationary vortex (of horizontal size  $1.5-2r_c$ ) of RDX combustion products to form in a wave structure. Moreover, the gas entering the shock front through a central portion of the channel has to flow about the vortex, thus declining from the axis of symmetry towards a near-wall region.

Thus, it is demonstrated for the first time that within a certain range of parameters ( $Y_{10} \leq 0.333$ ) the self-sustaining stationary DW with a vortex structure was formed in a cylindrical channel. When engulfing particles coming through the leading front, the vortex of hot gaseous products provides heating and ignition of the particles. That is, with decreasing initial gas pressure  $p_0$  (decreasing  $Y_{10}$ ), transition from the shock-induced to convective mechanism of HE particles ignition occurs. The latter is realized as a vortex of hot products in the reaction zone structure of DW.

## PECULIARITIES OF A DETONATION OF NITROBENZENE AND PROPYNOL

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A criterion dividing explosive and non-explosive substances in explosion safety regulations is rather conditional in some sense because of its strong dependence on conditions of initiation and propagation of explosive transformation. Thus, the systems exhibiting weak explosive properties are of interest for both theoretical studies and practical development. Some organic nitrocompounds which have one nitrogroup and three or more carbon atoms as well as some acetylene derivatives belong to these systems in spite of being generally considered to be relatively safe.

This paper presents the results of investigation of detonation propagation conditions in liquid substances, nitrobenzene ( $C_6H_5NO_2$ ) and propynol ( $C_3H_4O$ ). Estimated heat of explosion of nitrobenzene (at maximal density) is  $Q = 4$  MJ/kg, and of propynol is  $Q = 4.3$  MJ/kg. These heats are a little less than the corresponding value for dinitrotoluene (4.5 MJ/kg). In our previous work, detonability of melted dinitrotoluene was shown to grow essentially with porosity. Taking this fact into consideration, the influence of porosity on detonability of both nitrobenzene and propynol was studied experimentally.

The experiments were carried out in steel tubes (diameter  $d = 10$  mm, wall thickness  $h = 13$  mm, length  $L = 250$  mm). To register the process by means of streak camera (GFR-3), radial holes ( $d = 2$  mm, with spacing 25 mm) were drilled in a tube wall. For reducing the density of a nitrobenzene charge, it was gelled by adding colloxylin (5%) and, after addition of a small amount of surfactant, intensively mixed at  $T \sim 50$  °C. For preparation of porous propynol charges, the tube was first filled with porous polystyrene spheres (diameter 2.5–3.5 mm) and then with propynol. At the top of the tube, a fine mesh wire gauze was mounted to prevent flotation of the porous spheres.

Experimental detonation velocity of nitrobenzene at density of 0.5–0.7 g/cm<sup>3</sup> is 0.8–1.1 km/s, while that of propynol (at  $\rho = 0.43$ –

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0.44 g/cm<sup>3</sup>) is 2.2–2.3 km/s. Detonation velocity of nitrobenzene is 25–50% lower than the ideal detonation velocity calculated by using the SD computer code.

The heated and burned fractions of the detonating substance, the conditions of steady state detonation propagation, and the values of critical porosity were calculated for both the substances. The theoretical results correlate well with the experimental findings.

## SHOCK COMPRESSION OF LIQUID HYDRAZINE. ESTIMATION OF DETONABILITY AND SENSITIVITY TO SHOCK LOADING OF ITS SOLUTIONS

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The paper shows a method of calculating the parameters of shock compressed liquid hydrazine within the framework of the approaches developed for studying shock compression of organic liquids and liquefied gases. In the case when the mass velocities behind shock fronts do not exceed  $3.1 \text{ mm}/\mu\text{s}$ , it may be managed under assumption of the retention of the initial compound (hydrazine) behind a shock front. Detonation velocities of hydrazine solutions with such explosives as nitromethane and hydrazinenitrate correspond to destruction of hydrazine to ammonia and nitrogen, which is accompanied by a noticeable energy release. The estimates demonstrate a possibility of detonation of liquid hydrazine at the velocity of  $8 \text{ mm}/\mu\text{s}$  with shock heating of the liquid to approximately  $2000 \text{ K}$  which is comparable with the temperature observed behind a shock front during detonation of liquid explosives. Large values of the critical diameter of detonation (up to  $1 \text{ m}$ ) are expected because of a large activation energy of hydrazine decomposition ( $53.2 \text{ kkal/mol}$ ) which is almost 1.4 times larger than the activation energy of decomposition of standard explosives. In this case, their more rapid decomposition behind a shock front results in temperature increase that is sufficient for hydrazine destruction for time less than  $0.1 \mu\text{s}$ .

## THERMODYNAMIC MODELING OF DETONATION PARAMETERS OF FUEL-AIR MIXTURES

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Air shock waves generated by unconfined detonation of combustible aerosol or dust clouds may cause a strong damage. In accidental situations, an explosion may be initiated in clouds of complex composition with high energy effective fuels. Experimental determination of detonation parameters of such systems is difficult. Therefore, estimates of the effect of composition of combustible mixture on the detonation parameters and the blast waves produced in air are of great interest.

The equilibrium thermodynamic calculations of detonation and isentropic expansion of detonation products were carried out to find the effect of addition of effective high energy fuels to mixture on the parameters and performance of unconfined detonation. The equation of state (EOS) of an ideal gas and the virial EOS were used for thermodynamic calculations of detonation of fuel-air mixtures and dust or aerosol mixtures of explosives with negative oxygen balance. Aluminum, *n*-propylnitrate, nitromethane and many other substances were considered as energy effective fuels. It was shown, that detonation pressure increases with the number of gaseous moles per kg of products. A relation between the detonation pressure and the internal energy of the products expanding to ambient pressure was obtained which allows to estimate the performance of these systems.

The strength of a blast wave at large distances from the unconfined detonation may be estimated from the energy balance based on thermodynamic considerations. The estimates of the effect of the explosion mode on the shock waves produced in the air have been made. It was shown that the energy transferred to the ambient surroundings is minimal for combustion at low flame speeds and maximal for detonation initiated in the cloud center. At large distances, any mode of explosion (single- or multi-stage) produces a blast wave whose amplitude is less than that of the relevant Chapman-Jouguet detonation.

## THERMODYNAMIC MODELING OF DETONATION OF LIQUID EXPLOSIVE MIXTURES CONTAINING HYDRAZINE

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Liquid explosive mixtures containing hydrazine are used in rockets as components of propellants and in other technical devices. Detonability of the mixtures are investigated less than the detonation properties of individual components. Therefore, theoretical determination of detonation parameters of the liquid explosive mixtures is of great importance for predicting their detonation behavior.

In this work, thermodynamic calculations of detonation parameters of binary (hydrazine–nitromethane) and ternary (hydrazine–nitromethane–methanol) mixtures were carried out.

For describing thermodynamic properties of gaseous detonation products, the BKW equation of state (EOS) with the authors own set of coefficients, BKW–RR, was used. Previously [1], this EOS has been successfully applied to thermodynamic modeling of detonation for a number of solid CHNO-explosives. Two solid carbon phases (graphite and diamond) were considered as possible condensed detonation products.

The calculated detonation velocities are in satisfactory agreement with available experimental data. It has been shown that solid carbon is presented in detonation products of the most studied mixtures in the form of small carbon clusters. At some compositions of the mixtures, the calculations predict the anomalous detonation mode [2], that causes abrupt change in the slope of the detonation velocity vs. mixture composition curve and the corresponding discontinuities in pressure values behind the detonation front. In addition to molecules of hydrazine and nitromethane, the hydrazine–nitromethane binary mixtures were found to contain associate molecules, resulting from chemical reactions between hydrazine and nitromethane. The presence of the associate molecules in the hydrazine–nitromethane solution yields the observed minimum in the dependence of detonation velocity on

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hydrazine concentration and allows to explain why the experimental shock sensitivity of this binary system attains maximum at hydrazine concentration of about 25 weight-percent.

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## INTERPHASE HEAT AND MASS TRANSFER IN A CHEMICALLY REACTING BUBBLE MEDIUM

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This paper presents a solution of the problem on dynamics of a single bubble in a liquid with external pressure, chemical reactions, intensive inter-phase heat and mass transfer, and soot formation taken into account. This work is considered as a stage in creating an adequate model of bubble detonation (including cases, where fuel and oxidizer are in different phases) and of detonation initiation in complex heterogeneous systems.

Realistic heat and mass transfer processes are modeled by instantaneous (at time moment  $t_{inj}$  after beginning the compression) evaporation of mass  $M_L$ . Heat and mass transfer between phases is taken to be zero during the subsequent evolution of the system. Bubble dynamics is described by the commonly accepted model, where a bubble is supposed to have a spherical shape, the gas is ideal, and chemical reactions occur in the gas phase. It is assumed, that the state of a vapor-gas mixture at the end of induction period  $t_i$  corresponds to a non-reactive gas, and after the induction period it is in chemical equilibrium. Thermodynamic parameters of the mixture are calculated according to the approximate kinetic model [1, 2] without using the inert gas adiabat.

This model is applicable to hydrogen-oxygen systems of arbitrary composition (including those containing inert components and soot). This allows to consider adequately the drastic change in the molecular weight, the ratio of specific heats, specific heats, and the heat effect of chemical reaction due to recombination and dissociation processes and due to variation of the fuel-oxidizer ratio in the gas phase. For instance, for the initially cryogenic mixture (1)  $H_2$  (gas) -  $O_2$  (liquid), the molecular weight of gas can vary by an order of magnitude.

The proposed model was applied for simulating the bubble dynamics depending on  $t_{inj}$  and  $M_L$  in systems (1) and (2)  $[2H_2 + O_2$  (gas) -

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H<sub>2</sub>O (liquid)] with and without inert diluant and soot. The dependence of gas parameter  $M_L$  for mixtures (1) and (2) was shown to be considerably different. For example, in system (1) with increasing  $M_L$  the average gas temperature in a bubble passes through a maximum, while in system (2) increasing  $M_L$  leads to monotonous decrease in the gas temperature. The conditions are found when there exists a considerable dependence of the process dynamics on  $t_{inj}$ . The influence of inert diluants is analyzed.

Increase in argon concentration in a bubble results in the growth of the final temperature in system (1) and its decrease in system (2). Internal pressure and compression ratio decrease in both cases, and the temperature increases during the first pulsation.

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## PECULIARITIES OF OXIDATION OF ALUMINUM PARTICLES IN DETONATION PRODUCTS OF HETEROGENEOUS EXPLOSIVE SYSTEMS

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Studied in this work is thermodynamics and macrokinetics of oxidation of dispersed aluminum in shock and detonation waves propagating in heterogeneous energetic materials. The analysis is carried out by applying both the methods of equilibrium chemical thermodynamics and hydrodynamics of reacting media.

Specific features of aluminum behavior in detonation of heterogeneous explosive systems with different characteristics: high density explosives (HMX, RDX, TNT), oxidizers (perchlorate, nitrate, etc.), porous (solid and liquid) compositions, gaseous systems and aerosuspensions — are considered. Comparison of numerical and experimental data shows that the state of dispersed aluminum at the Chapman-Jouguet point and its influence on the detonation parameters is qualitatively different for charges of different density (high, porous, low) and oxidizing balance (positive, negative). Thermodynamic conditions for the formation of intermediate products of aluminum oxidation including the condensed oxide  $\text{Al}_2\text{O}_3$ , were investigated. The comparative analysis of Hugoniot and rarefaction isentropes of equilibrium and partially 'frozen' reaction products at the  $P$ - $V$  plane was also made.

The thermodynamic features of metal combustion were used in numerical simulation of shocks and detonations propagating in reacting media with double-stage energy release. Thus, the effect of macrokinetics of aluminum oxidation on the flow patterns can be determined by applying a combined multi-purpose method based on experimental and numerical approaches. Based on the analysis of experimental data, the approximations were proposed for the rate of oxidation of aluminum powders of various dispersity. The problem of constructing the model of aluminum oxidation kinetics at high pressure is discussed.

## NUMERICAL STUDY OF TRANSIENT PROCESSES DURING COMBUSTION OF POROUS FUELS

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Convective combustion (CC) of a porous fuel is a combustion process propagating due to ignition of a cold fuel by forced convection of hot gas. The phenomenon of CC often occurs naturally and in technical devices. At elevated pressures, all porous combustible materials appear to burn according to this mechanism. Actually, the CC mode and the mode of low-velocity explosive conversion (LVEC) are the consequent stages of deflagration-to-detonation transition. The study of these processes is important for avoiding anomalous effects associated with the use of porous fuels and for explosion safety. The paper presents a mathematical model describing transition of CC to detonation in a porous fuel which is considered as a visco-plastic porous medium.

The model is based on the following assumptions. The initial porosity of a charge is allowed to be lower than gravimetric. All pores in a charge are connected. When porosity attains a certain specific value, the skeleton is dispersed to a set of identical particles, and the pressure of the dispersed phase is taken equal to the gas pressure. In the undispersed porous matrix, the pressures in phases are different. Since it is hardly possible to take into account geometric features of actual pores, the pores are simulated by effective cylindrical channels with equivalent volume and surface.

The model is based on the equations of motion and energy conservation for the gaseous and condensed phases, heat conductivity equation for pore walls, and additional relationships determining mass, momentum, and energy transfer between the phases. The set of equations is supplemented by the equation of deformation of an effective cylindrical pore, and the expressions for the radial velocity component of fuel particles and dissipated energy. For describing a temperature field in the condensed phase, two regions are considered: boundary and bulk. The former is a thin fuel layer near the pore wall with

the temperature distribution depending on the convective heat flux governed by the heat conductivity equation. The latter includes the rest of the fuel. In this region, only deformation-induced dissipative heating of condensed phase should be taken into account, and the influence of a convective heat flux can be neglected.

For implementing the model, a numerical procedure is developed. The governing equations were integrated by using the explicit conservative scheme of a Lax-Vendroff type on a moving adaptive grid. For demonstrating the capabilities of the model, CC of a granulated charge in a closed volume was simulated.

All combustion regimes, commonly observed in experiments, are detected in calculations: developed CC, stabilized CC and LVEC. The calculated values of ignition rates differ from measured by 12–15%. The analysis of thermal conditions at internal surfaces of pores indicates that, at the moment of transition from CC to LVEC, the change in the ignition mechanism occurs, from one governed by convective heat transfer to another governed by visco-plastic deformation of skeleton.

Numerical parametric studies of combustion of low porosity charges in closed volume are conducted. The influence of initial and rheological fuel properties such as porosity, specific surface, charge length, viscosity, and yield point, on combustion characteristics is investigated. Predictions are compared with available and authors own experimental data.

## EXPERIMENTAL METHODS FOR STUDIES OF COMBUSTION IN CONDENSED SYSTEMS

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Determining the laws of burning and gas formation in condensed systems is a necessary step towards the development of mathematical models of explosion processes. Limitations of experimental methods force scientists to search for indirect techniques to identify these laws.

The paper presents two experimental techniques aimed at identification of the burning and gas formation laws in condensed systems. The first allows, with a minimum additional assumptions, to establish the burning law and the burning surface for statistically monodispersed fuel samples. The second is designed for studies of the structure of convective combustion zone in low-porosity double-component monoblock charges, when the burning laws of both components are known.

In both cases, the test samples are burned in a closed (constant volume) chamber, and the only measurement is the pressure of combustion products vs. time. The experimental data are discussed and compared with the data of other researchers.

The use of suggested techniques allows to simplify essentially the determining of the burning and gas formation laws in condensed systems.

## OPTICAL METHODS OF DETONATION DIAGNOSTICS

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Many methods of optical diagnostics of physical processes (interferometric and shadow methods, polarimetry, some spectroscopic methods, etc.) provide simultaneous registration of two important characteristics of the object under study. The first is the capability of the method to register a signal emitted by the object surface (volume) as a whole. The second is that the registered signal is the integral of a certain characteristics of the object along the observation line. It is shown in [1-3] that these two features allow to develop new approaches to optical studies of ignition, combustion, gas dynamic flows, the processes of interaction of radiation with the matter, etc. The new approaches allow to measure a number of integral parameters of the processes. Among them is the total mass of the domain under study, the total thermal energy in it, the power of heat release due to chemical reactions, the rate of heat release, variation of the momentum of a non-stationary flow, the profile of heat release rate in the stationary combustion wave.

This paper discusses possibilities of applying the new approaches to studies of detonation initiation and detonation structure. The primary attention is paid to interferometric and shadow methods. Application of the new approaches for other methods, including non-optical techniques, are also discussed.

Presented are the results of experimental investigation of laser-induced ignition of gas and vapors as well as ignition of gas by electric spark, which serve as illustrations of traditional and new possibilities of interferometric and shadow methods. Among the characteristics which were obtained are the temperature and density fields at different stages of the ignition process, and the data on the power and rate of heat release during ignition.

The results are obtained by means of automatic processing of interferograms (decryption). The corresponding codes are operator-friendly. Further development of the new approaches will allow to widen

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the application of optical methods and to face new challenging tasks in experimental investigations of detonation processes.

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## THERMODYNAMIC SIMULATION OF THE DETONATION PARAMETERS IN POROUS HETEROGENEOUS ENERGETIC MATERIALS

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Studies of synthesis and properties of advanced energetic materials (EM), including the propellants for advanced propulsion systems based on detonations, necessitate the development of methods for apriori estimation of detonation parameters on the basis of minimal information about the elemental structure, enthalpy and density of explosive charges. These methods can be developed within the frame of a thermodynamic approach, based on the joint solution of the following equations:

- set of equations of chemical and phase equilibrium for gaseous and condensed components of detonation products (with thermal and calorific equations of state holding within wide ranges of pressures and temperatures);
- conservation equations of the hydrodynamic theory of detonation, supplemented with the conditions of detonation stability (Chapman-Jouguet (CJ) conditions).

This paper presents the modeling procedure developed in the N. E. Bauman Moscow State Technical University and the results of thermodynamic simulation of detonation parameters for 5 groups of porous EM, which range in density from 100 to 1000 kg/m<sup>3</sup>. These are:

- (1) low density individual powder EM;
- (2) mechanical mixtures based on RDX with inert frame-forming additives (mipora, phenolformaldehyde microspheres) and reactive high energetic additives like Al, inorganic oxidizers (ammonium nitrate (AN), ammonium perchlorate (AP), and potassium perchlorate);

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- (3) low density cast systems based on TNT-RDX alloys (with foamed polystyrene and Al);
- (4) foamed mixtures based on explosives (PETN, RDX, AN, AP, TNT-RDX) and polyurethane;
- (5) filled and hydrous mixtures based on AN, individual high explosives and colloidal powders.

Since the complete thermodynamic equilibrium of detonation parameters at the CJ plane for indicated heterogeneous EM can hardly be attained, four types of calculations were used: corresponding to (I) ideal, and (II, III, IV) non-ideal detonation regimes. Parameters of non-ideal regimes were determined assuming partial thermal and chemical non-equilibrium of detonation products. In case (II), Al additive is assumed non-equilibrium. In case (III) only decomposition of the most active components, e.g. RDX, was taken into account, while the other components (inorganic oxidizers, dispersed Al, low-density frame-forming additives) were considered non-reactive and compressed in the mixture with detonation products of RDX. In case (IV), Al and inert additives were considered non-reactive, while all explosive components (EM, oxidizers) were assumed to decompose to their final products. The latter were assumed to undergo no mixing with each other in the reaction zone of detonation wave.

The results of thermodynamic simulation were compared with experimental data (extrapolated for explosive charges of infinite diameter). The effect of specific additives on detonation of porous EM is also analyzed.

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